# Assessment of the oxygen reactivity in a gas storage facility by multiphase reactive transport modeling

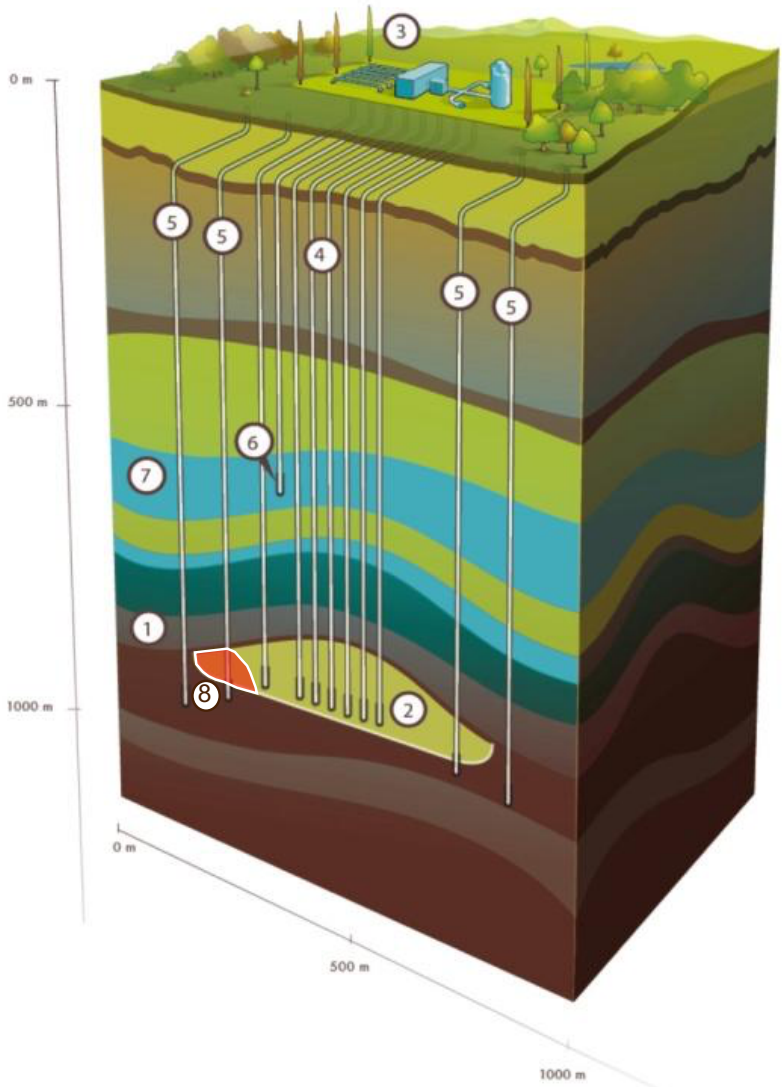
Irina Sin, Laurent De Windt, Camille Banc, Mines Paris, PSL University
David Dequidt, Anélia Petit, Storengy

Journée Thermodynamique du Sous-Sol SFGP, 12/07/2022

# Outline

# Context: aquifer gas storage facility

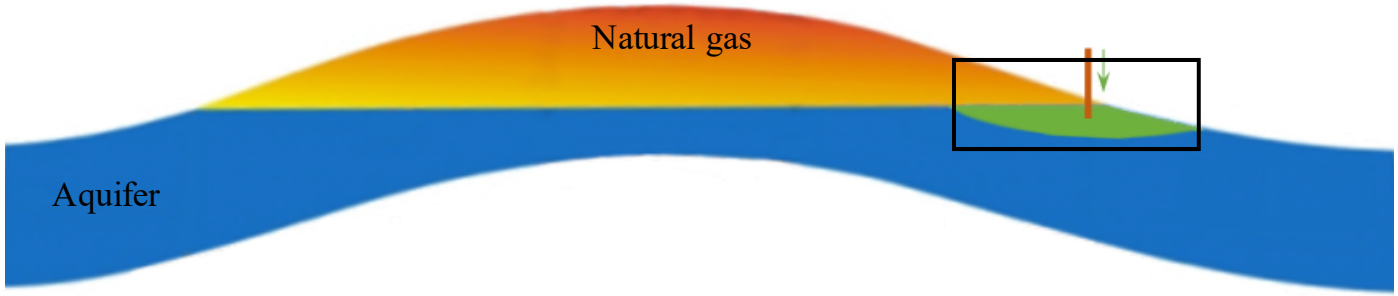
1) Caprock
2) Reservoir
3) Surface facilities
4) Injection and withdrawal wells
5) Monitoring wells
6) Monitoring wells of the upper aquifer
7) Upper aquifer
8) Cushion gas with $O_2$-depleted air




storengy

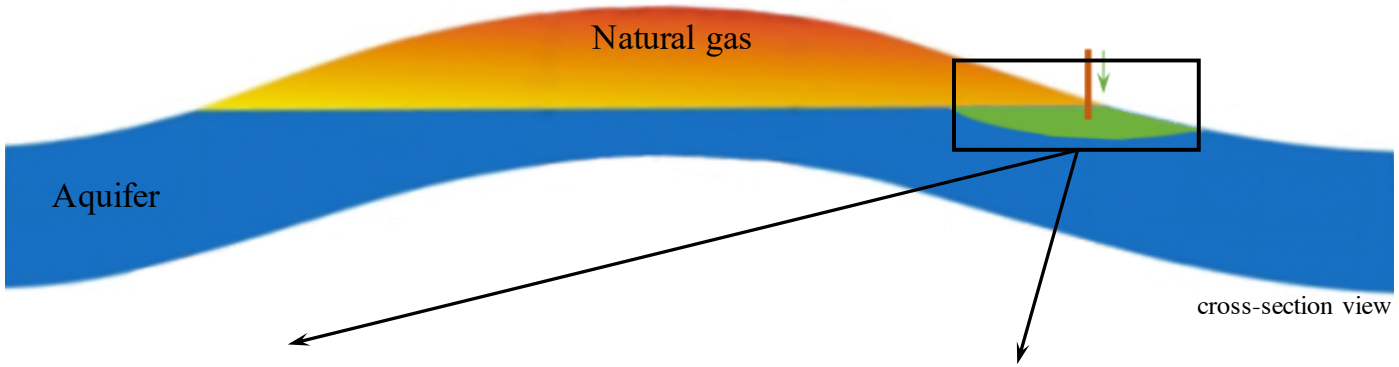
Une société de GDF SUEZ

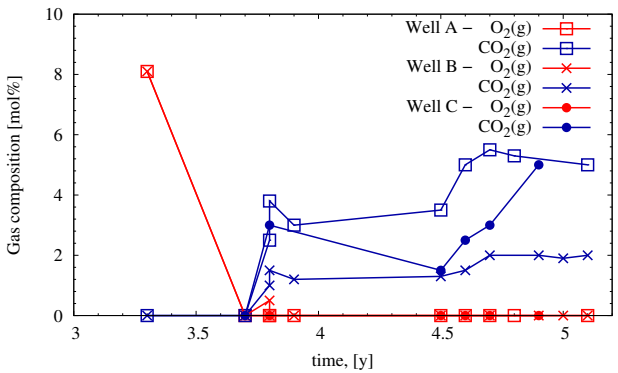
# Gas-water-rock interactions: observations

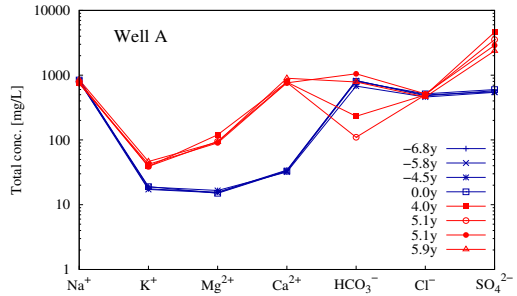


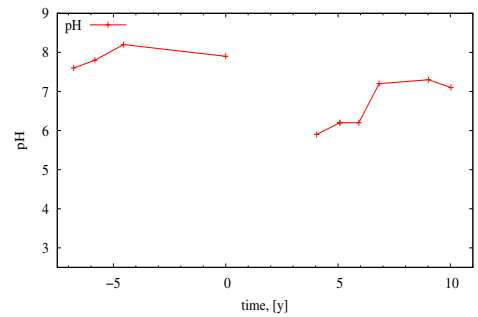

cross-section view

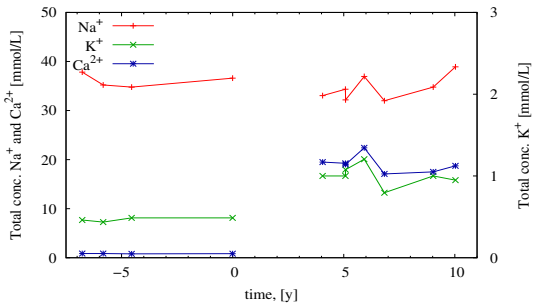
# Gas-water-rock interactions: observations

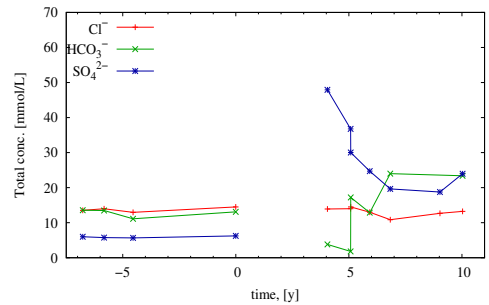


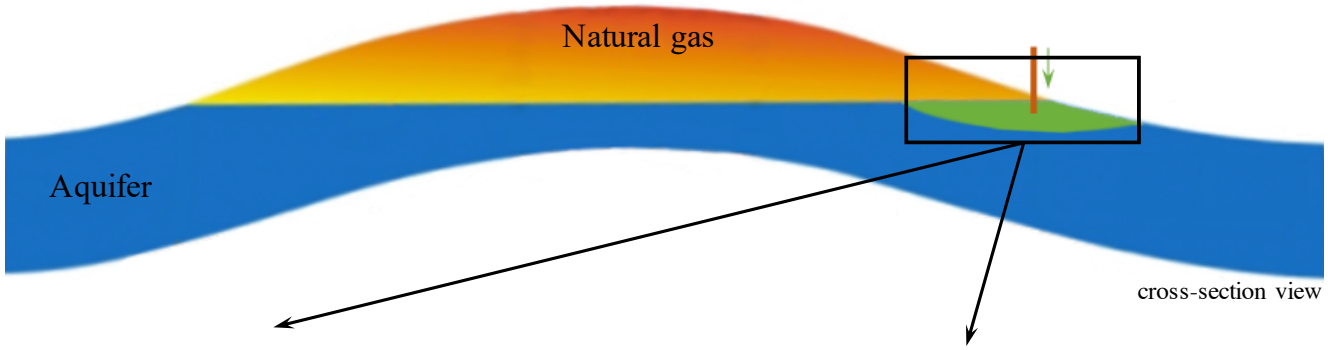



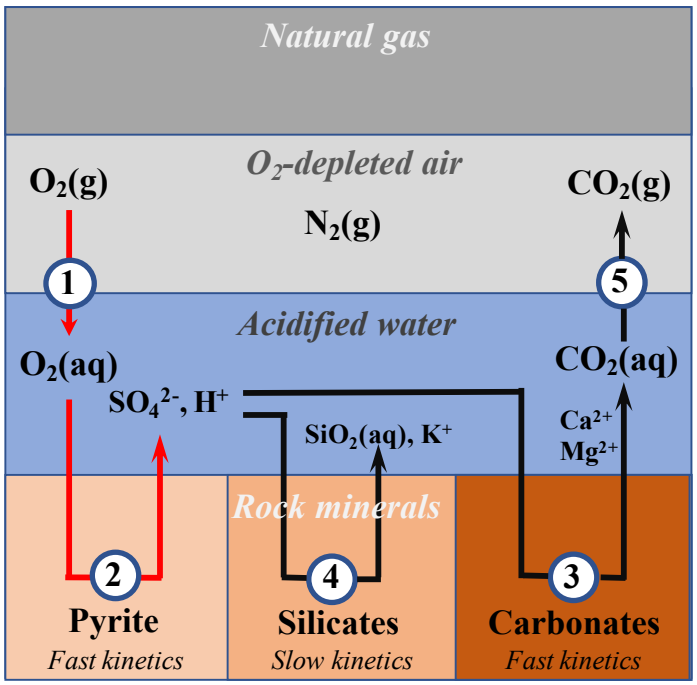




- What are the key mechanisms? What impact on the aquifer?

# Gas-water-rock interactions: model




- Cushion gas: $N_2$, Ar, $O_2$
- Phase equilibrium of gases + $H_2O(g)$

$$O_2(aq) \rightleftharpoons O_2(g)$$

- Pyrite oxydation

$$\text{Pyrite} + 3.75O_2(aq) + 2.5H_2O \longrightarrow \text{Goethite} + 2SO_4^{2-} + 4H^+$$

- Dissolution of calcite

$$\text{Caclite} + 2\,H^+ \longrightarrow Ca^{2+} + CO_2(aq) + H_2O$$

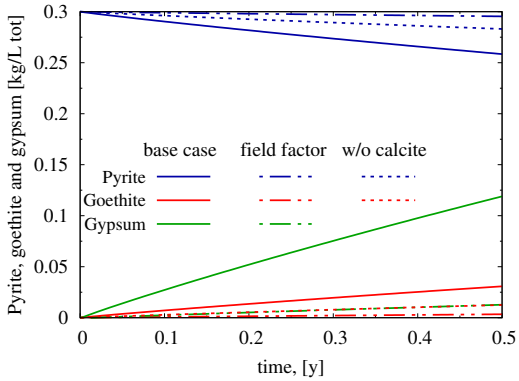
- Exsolution of $CO_2$

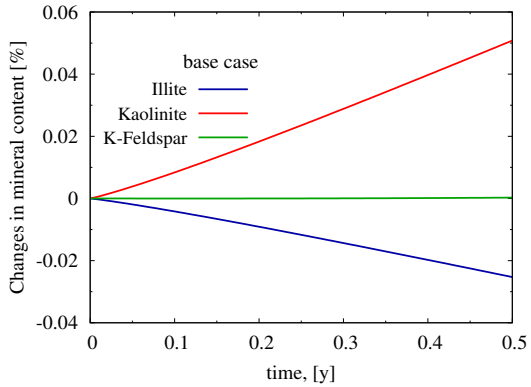
$$CO_2(aq) \rightleftharpoons CO_2(g)$$

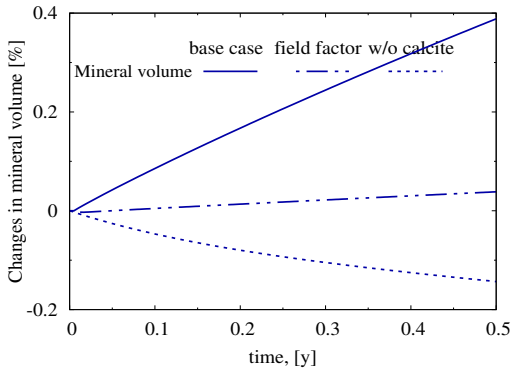
- What are the key mechanisms? What impact on the aquifer?

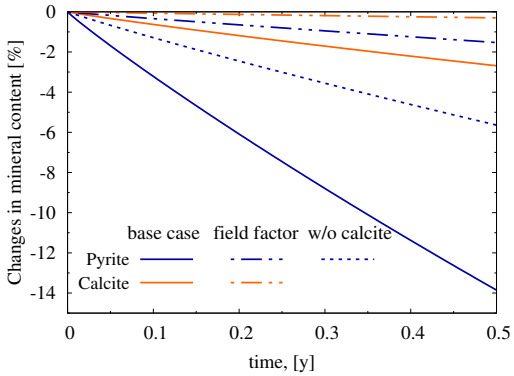
De Windt, Marsal, Corvisier, Pellegrini, Applied Geochemistry 41, 2014.

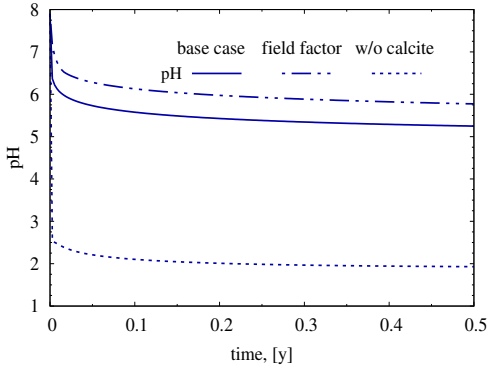
# Gas-water-rock interactions: batch results

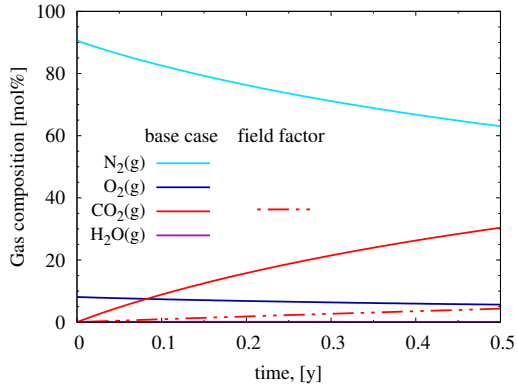


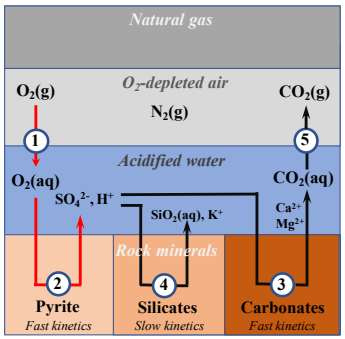



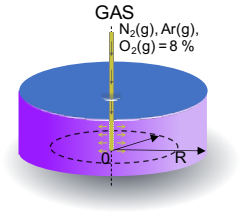



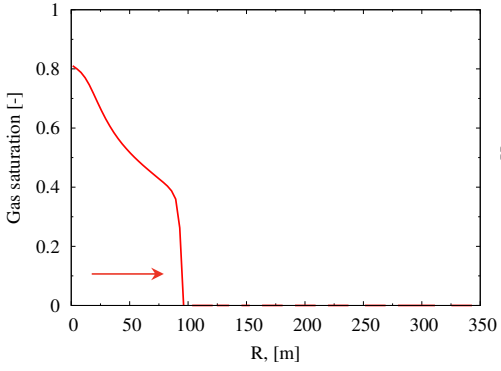



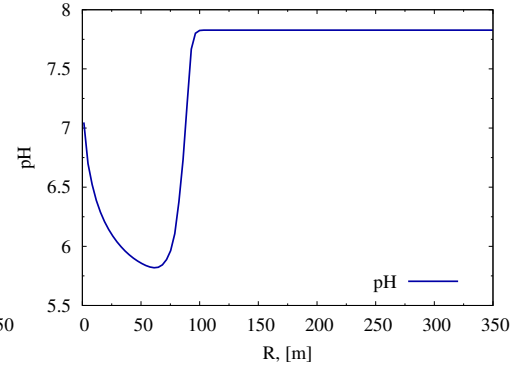

- Available data (borehole water sampling and gas composition before and after injection) are used to establish the model.
- Representation of major mechanisms vs site data
- Closed system → production of $CO_2$ is overestimated
- Reactive transport model is needed.

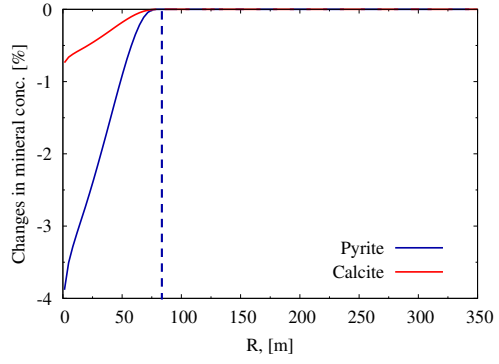
# Radial 1D multiphase reactive transport model

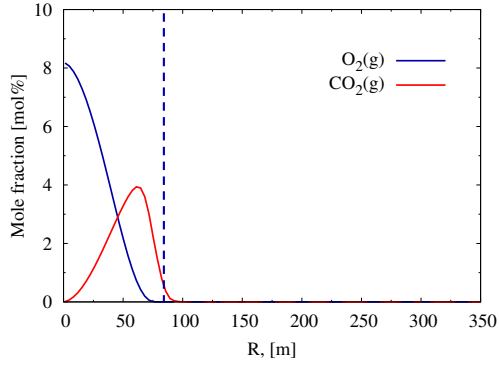



- 30 days

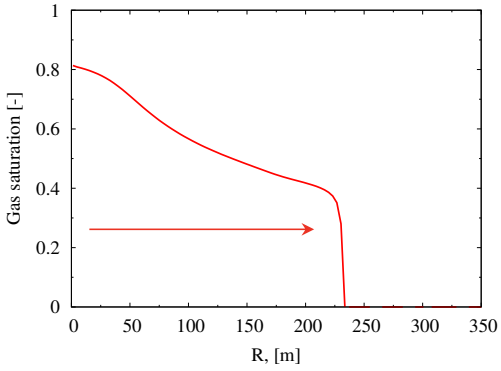


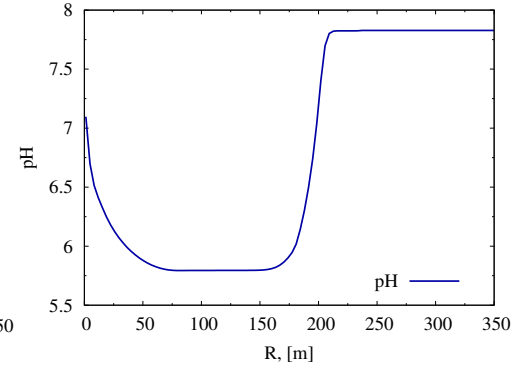



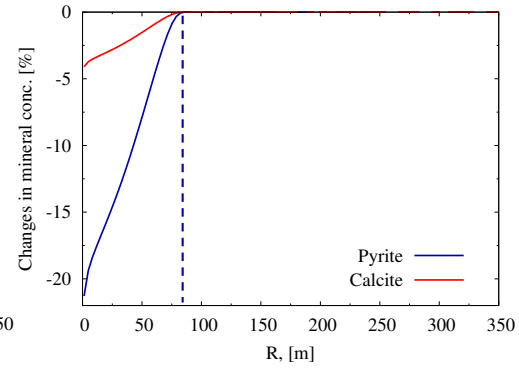



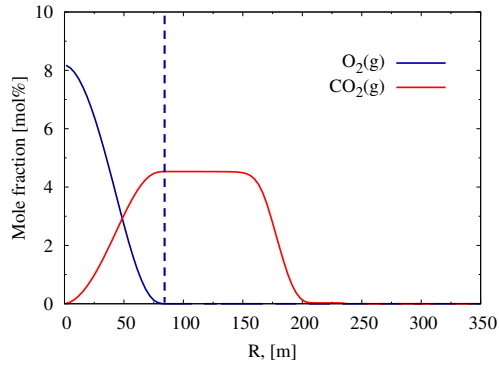




- 0.5 yr

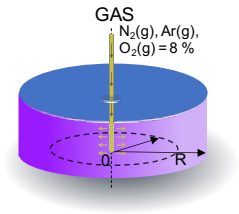


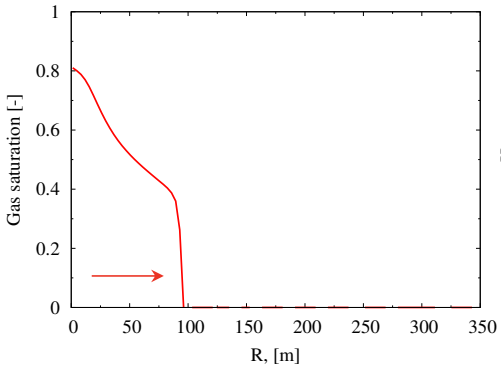



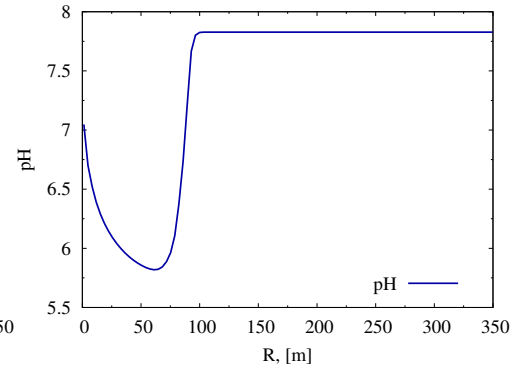



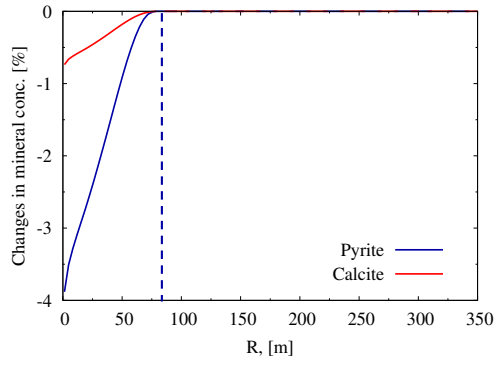
# Radial 1D multiphase reactive transport model

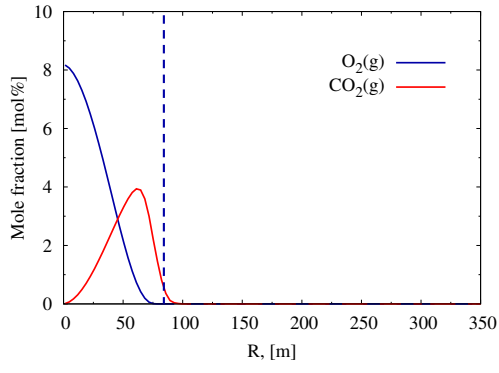



- 30 days

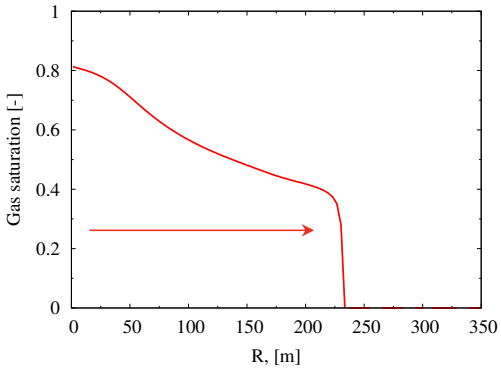


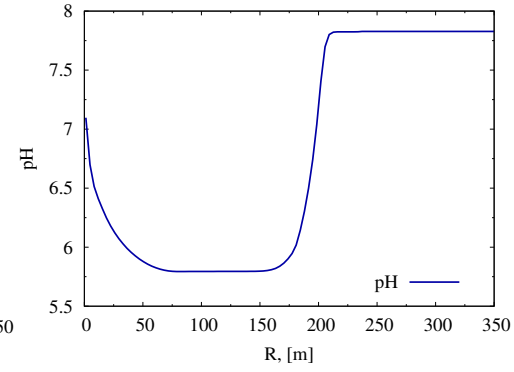



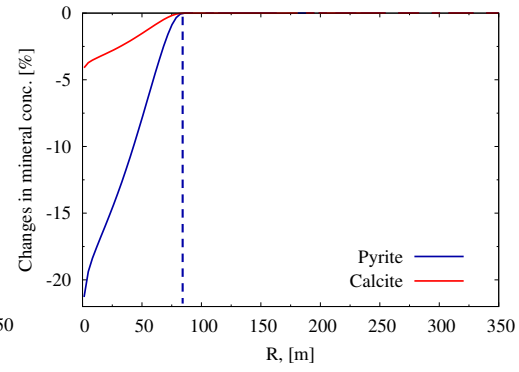



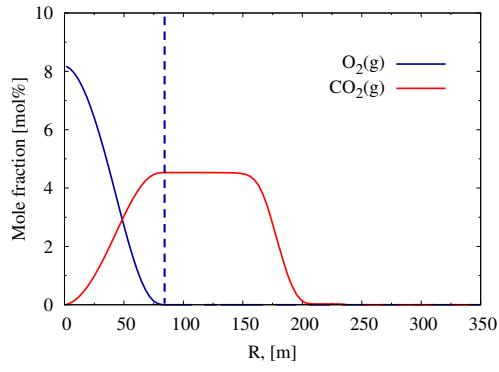




- 0.5 yr



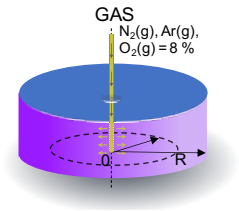



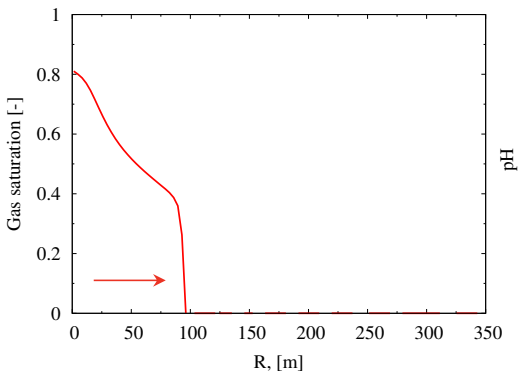



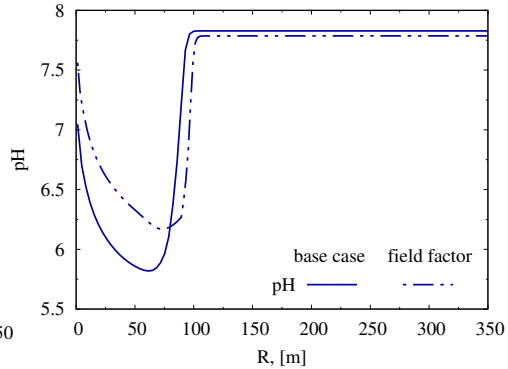

- Dissolution of pyrite/calcite → goethite/gypsum ↓
- ∼22% of pyrite is dissolved. Rapid $O_2$ consumption (same profiles at 30 d & 0.5 y).
- $CO_2$ accumulation grows with time, > 4 mol%.
- A slower kinetics is needed.

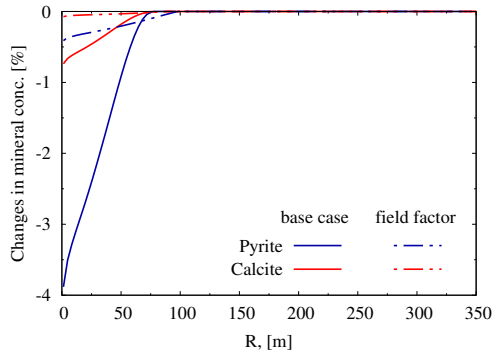
# Radial 1D multiphase reactive transport model: field factor

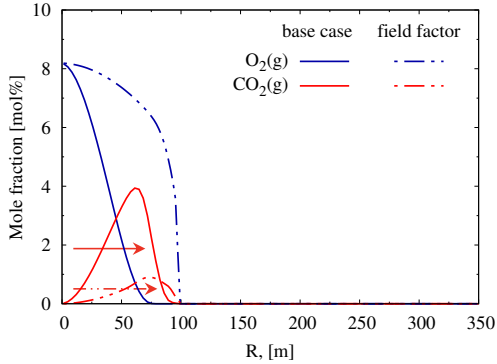



- 30 days

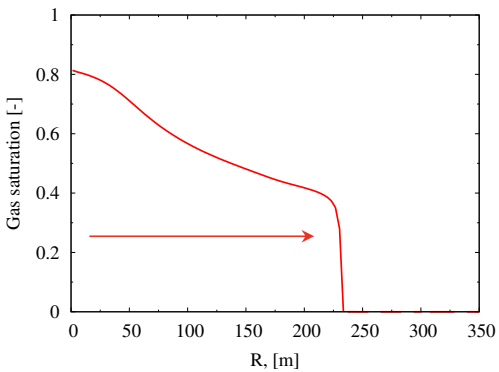


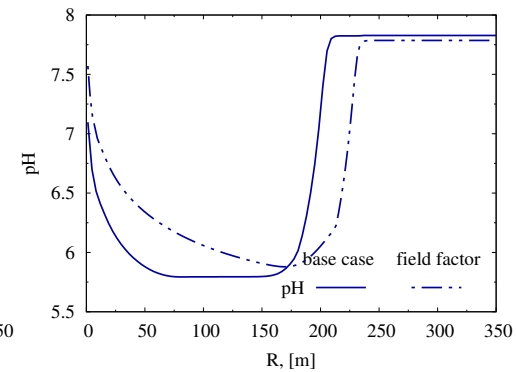



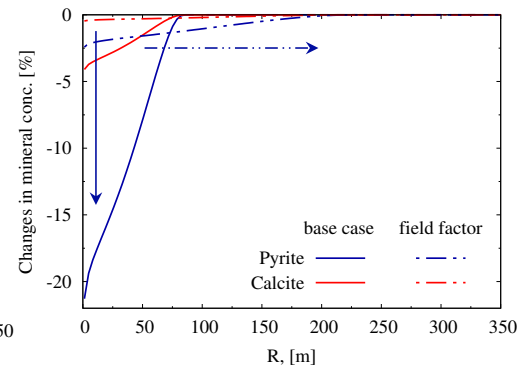



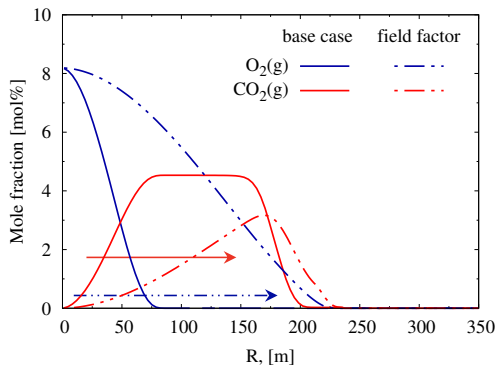




- 0.5 yr



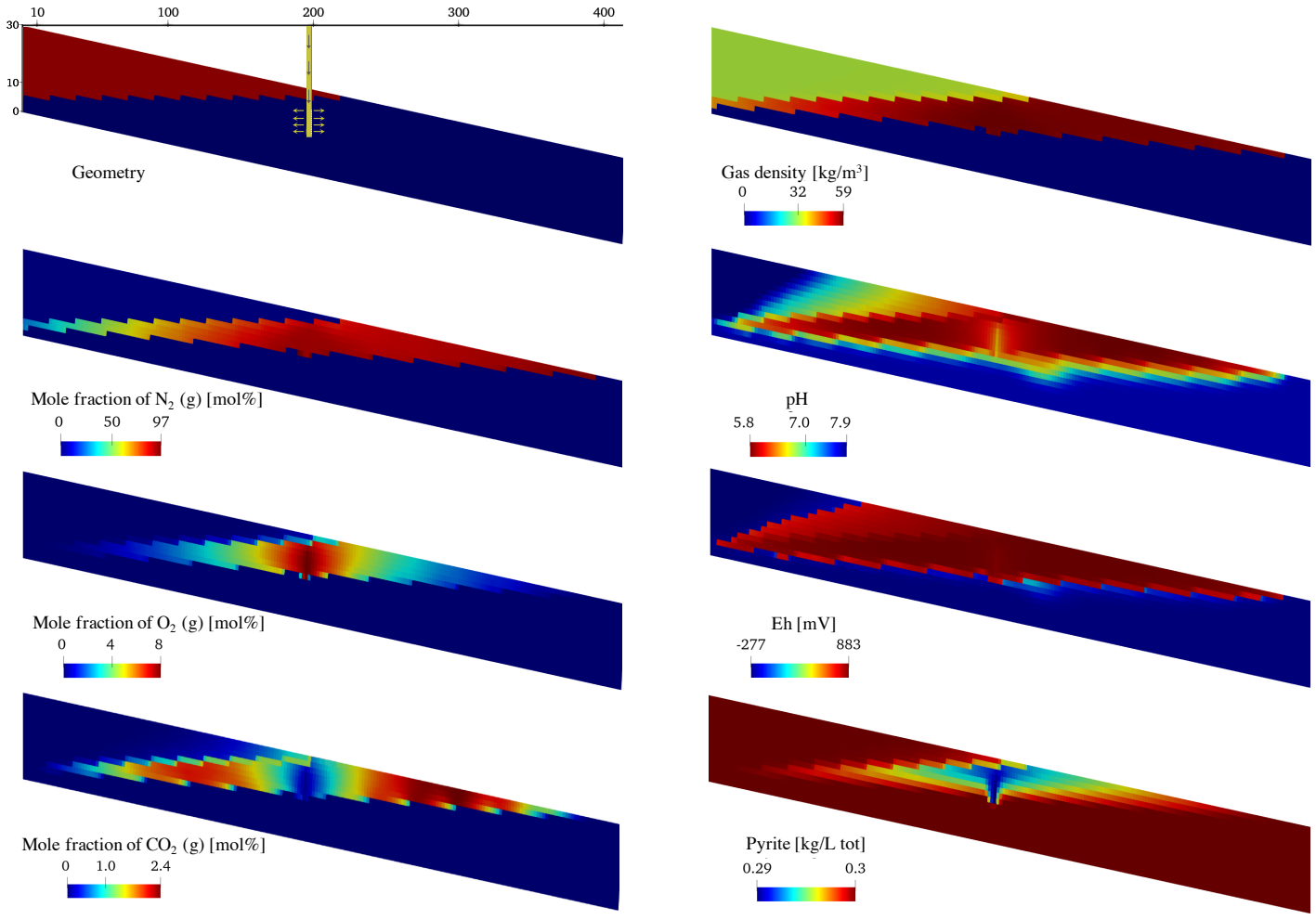




- Slower kinetics → ∼2% of pyrite is dissolved.
- Slower $O_2$ consumption → $O_2$ can be transported further → pyrite oxydation not only at near-wellbore zone
- $CO_2$ accumulation still grows with time, ∼ 3 mol%.
- Radial 2D reactive transport model is needed.

# Radial 2D multiphase reactive transport model

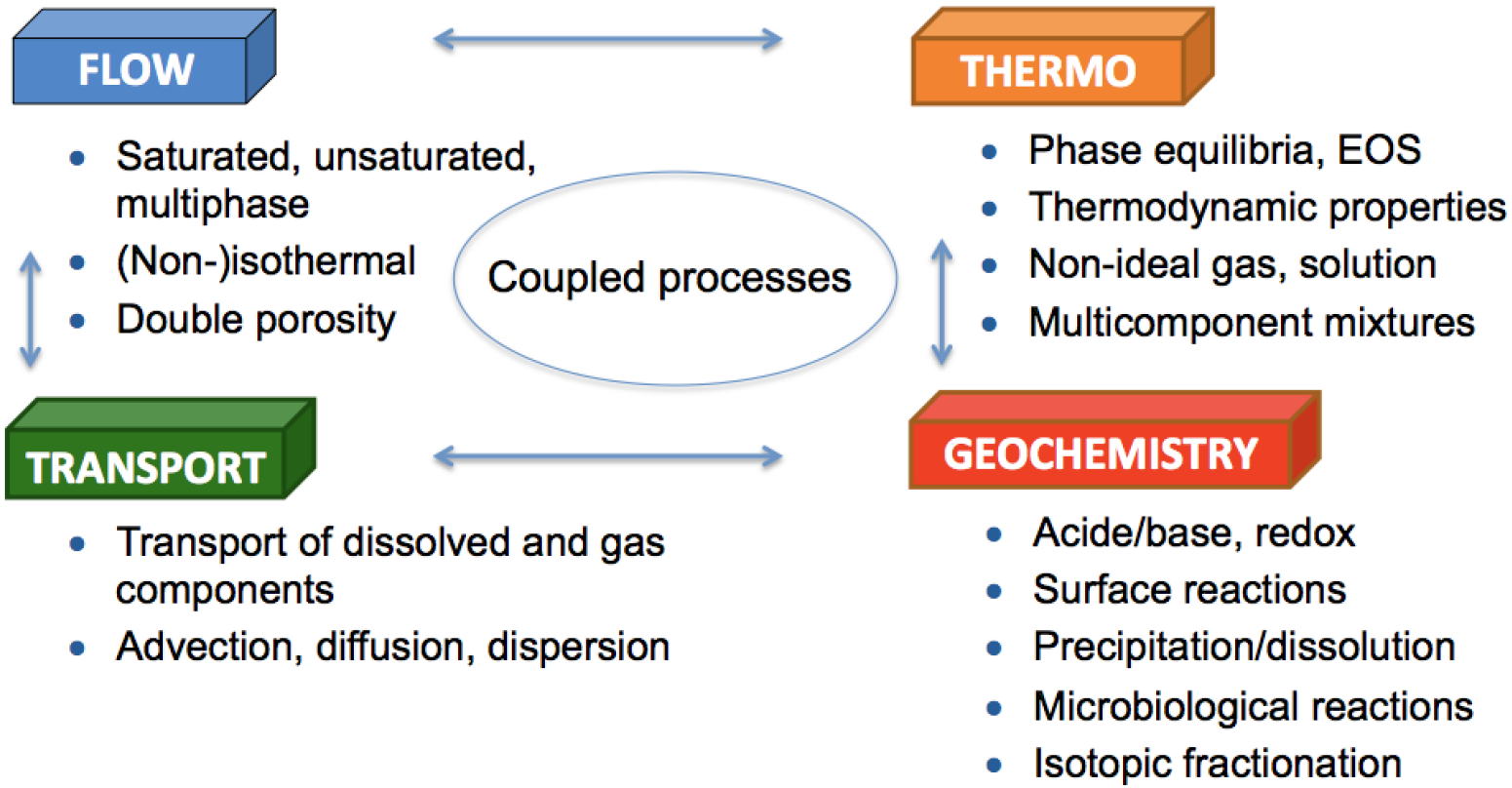
- 180 days




Sin et al (2022, submitted)

# HYTEC reactive transport code

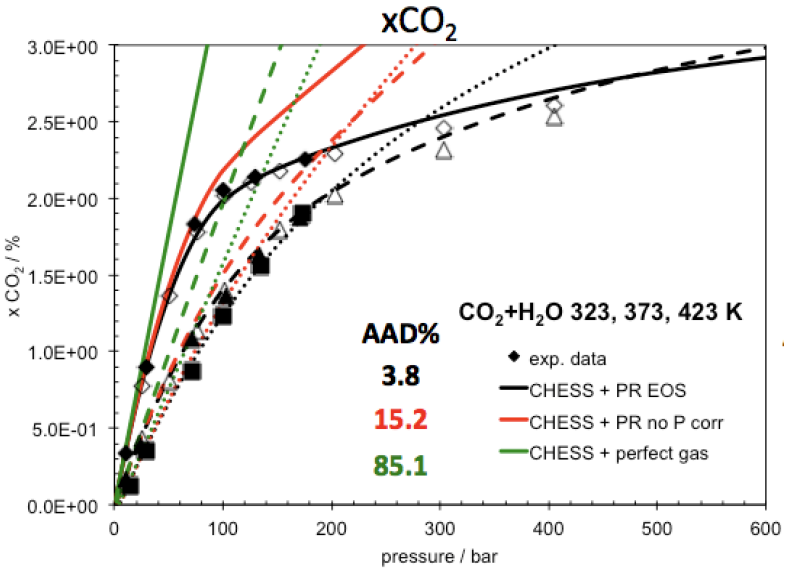
What physical and chemical processes?




van der Lee et al., Computers & Geosciences, 2003

# Solubility of real gases

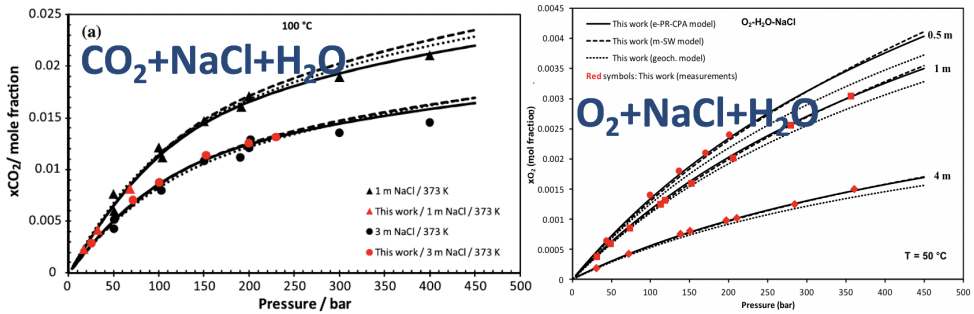
Fugacity – activity approach for gas-water-salt-rock systems




Data are required!

Experimental laboratory Géosciences/CTP

Measurements of thermophysical properties



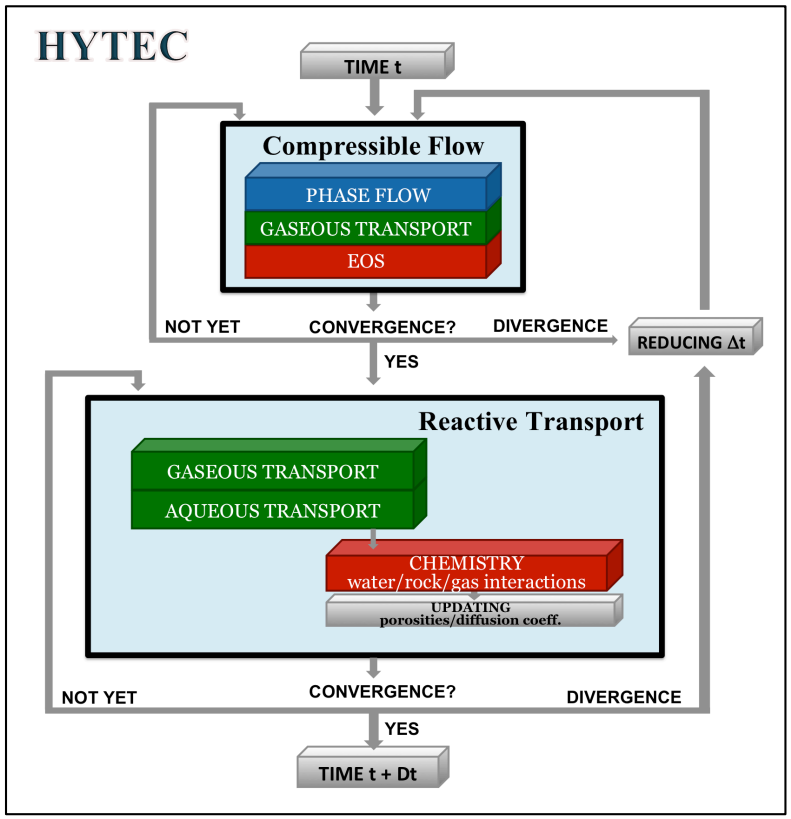

- $K^H$, BIP and EOS parameters adapted to non-ideal gases regarding $P$ and $T$.
- Helgeson-Kirkham-Flowers eq. for apparent molar volume; b-dot, SIT models.
- Analytical solution for the PR-type EOS models.
- Group contribution structure, easy application for mixtures.
- ANR GAZ ANNEXES, SIGARRR, FLUIDSTORY

Corvisier et al., GHGT-11 2013, GHGT-12 2014. Chabab 2021.
Corvisier&Sin, GHGT-14, 2018. Sin&Corvisier, RiMG 85, 2019.

storengy Une société de ENGIE MINES PARIS | PSL

# Reactive multiphase flow

## Reactive transport and geochemical speciation codes since 1999



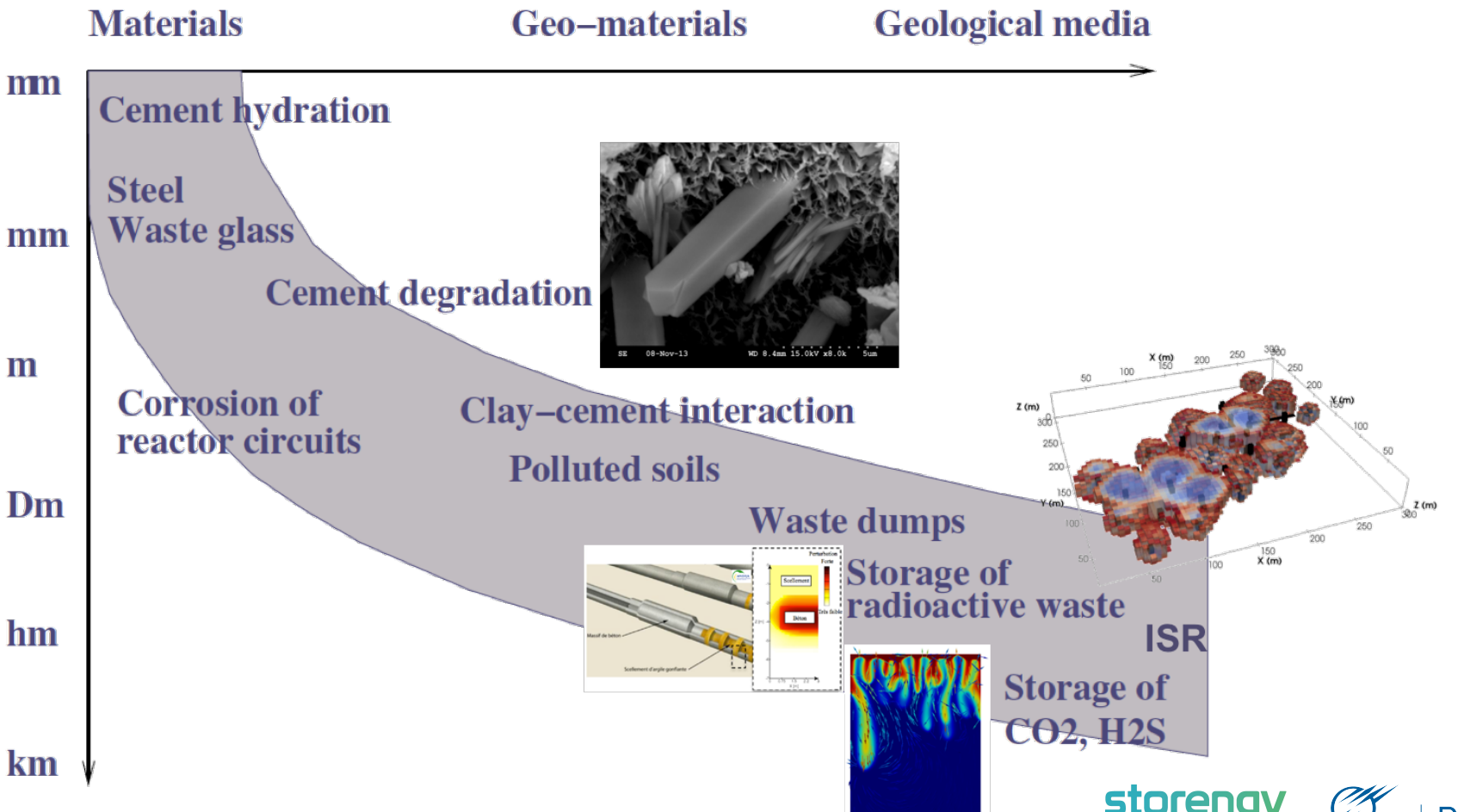

Coupling methods

- Operator splitting
- Flexibility
- CHESS
- Multiphase reactive transport
- Real mixtures
- Fluid properties

Sin, Lagneau and Corvisier, Adv. in Water Resources 100, 2017.

# HYTEC reactive transport code

What applications?



# Consortium PGT



Since 2000, **PGT**

- shared funding
- shared scientific research
- shared expertise

**PGT V** 2020 - 2023

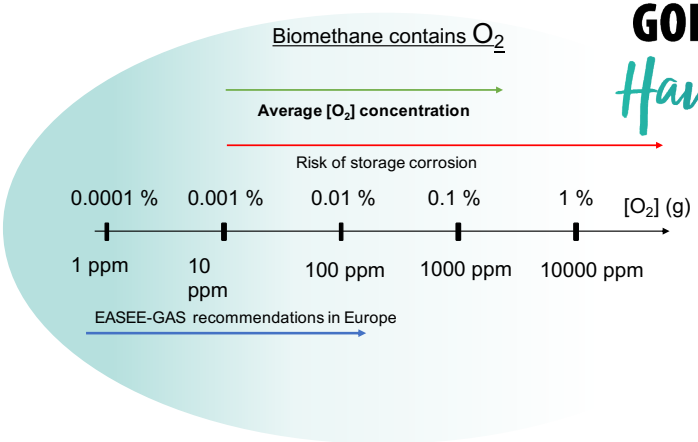
storengy Une société de ENGIE MINES PARIS | PSL

# Assessment of the oxygen reactivity in a gas storage by multiphase reactive transport

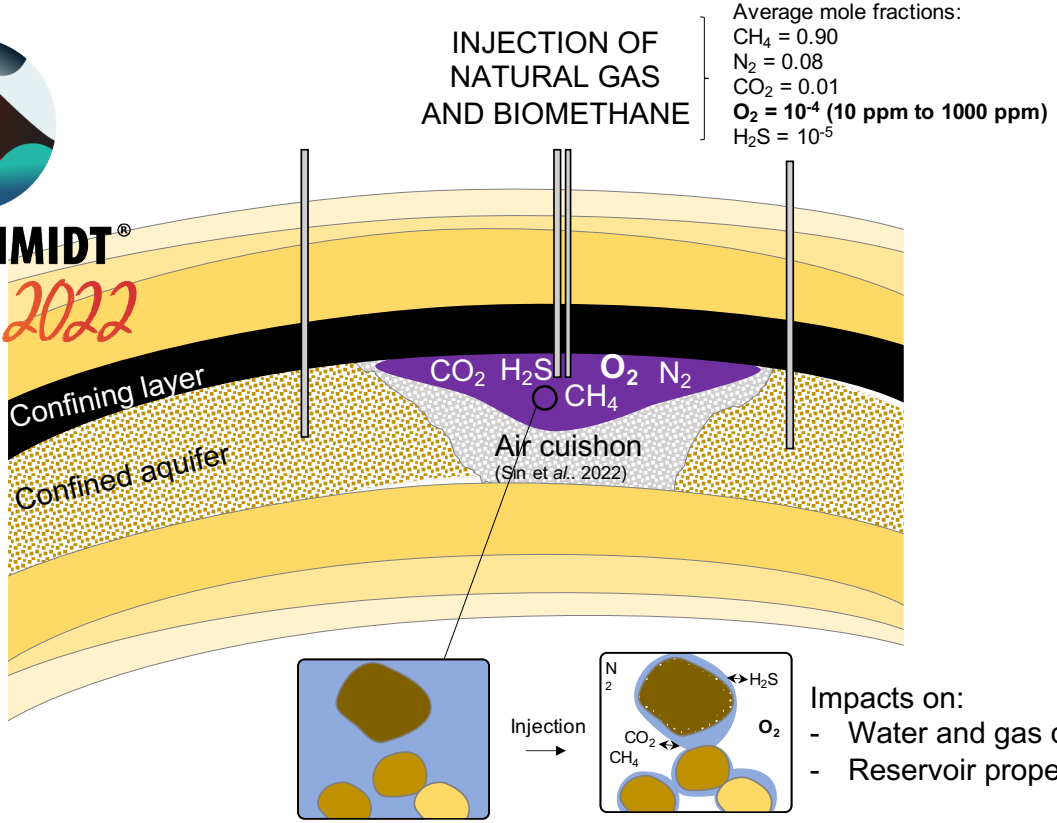
- 10 yr field data shows effects of injecting $O_2$-depleted air into aquifer gas storage: oxygen depletion, $CO_2$ appearance, pH decreases from 8 to 6 returning to the initial state after 3 years.
- Data were analyzed and the multiphase reactive transport model was built based on the field data. From batch to reservoir scales.
- Gas-water-rock reactive sequence was reproduced by the model: oxydation of pyrite, acidification, calcite buffering, gypsum and goethite precipitation, $CO_2$ exsolution.
- Pyrite kinetics is a significant factor. Damköhler number derived for $O_2$ reactivity and pyrite kinetics explains gas changes.
- The developed model could be used as a workflow for gas storage facilities (e.g., biomethane, compressed air, and $CO_2$).

# On-going work

Camille Banc, Multiphase reactive transport modeling of oxygen effect on deep gas storage aquifers, 12 July 2022




GOLDSCHMIDT® Hawai'i 2022




Impacts on:
- Water and gas quality
- Reservoir properties