COMSOL CONFERENCE
ROTTERDAM2013

AMPHOS 21
SCIENTIFIC AND STRATEGIC ENVIRONMENTAL CONSULTING

Reactive transport and convective mixing during CO_2 migration in a saline aquifer

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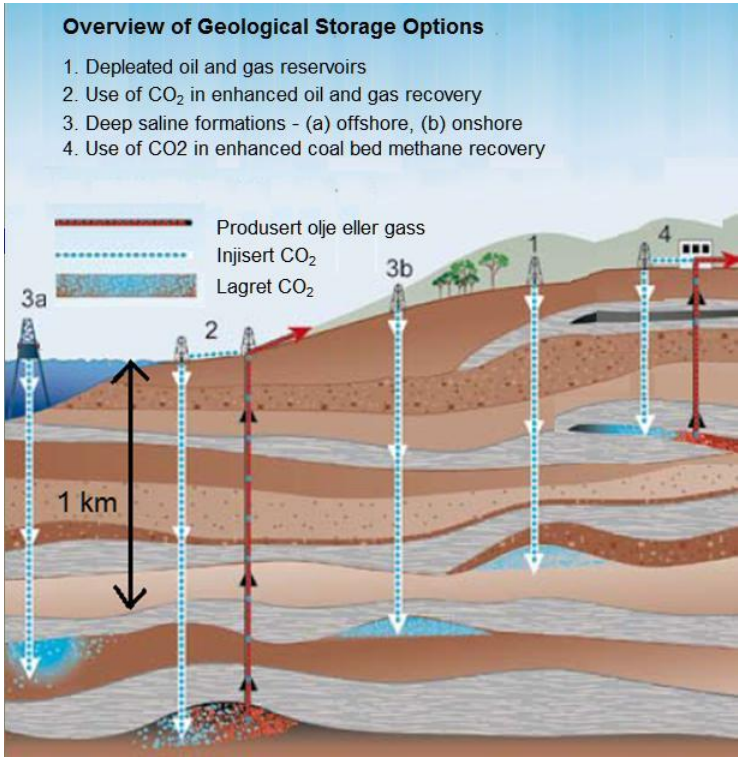
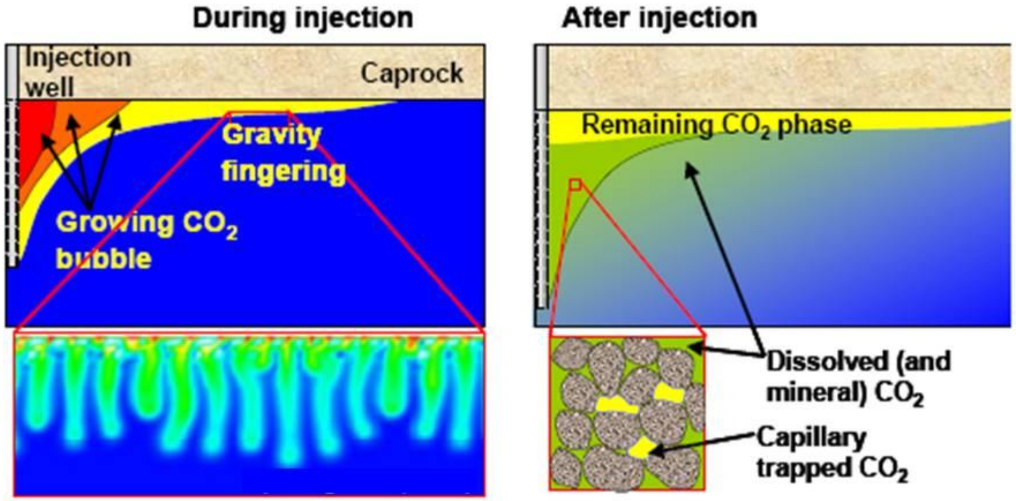
The problem

The conventional concept of CO_2 geological storage consists of injecting supercritical CO_2 into a saline aquifer at a sufficient depth so that the CO_2 has a high density (about 800 kg/m^3) and therefore occupies a reduced volume. This requires pressures higher than 80 bars, which explains that injection must be carried out at depths greater than 800 m.

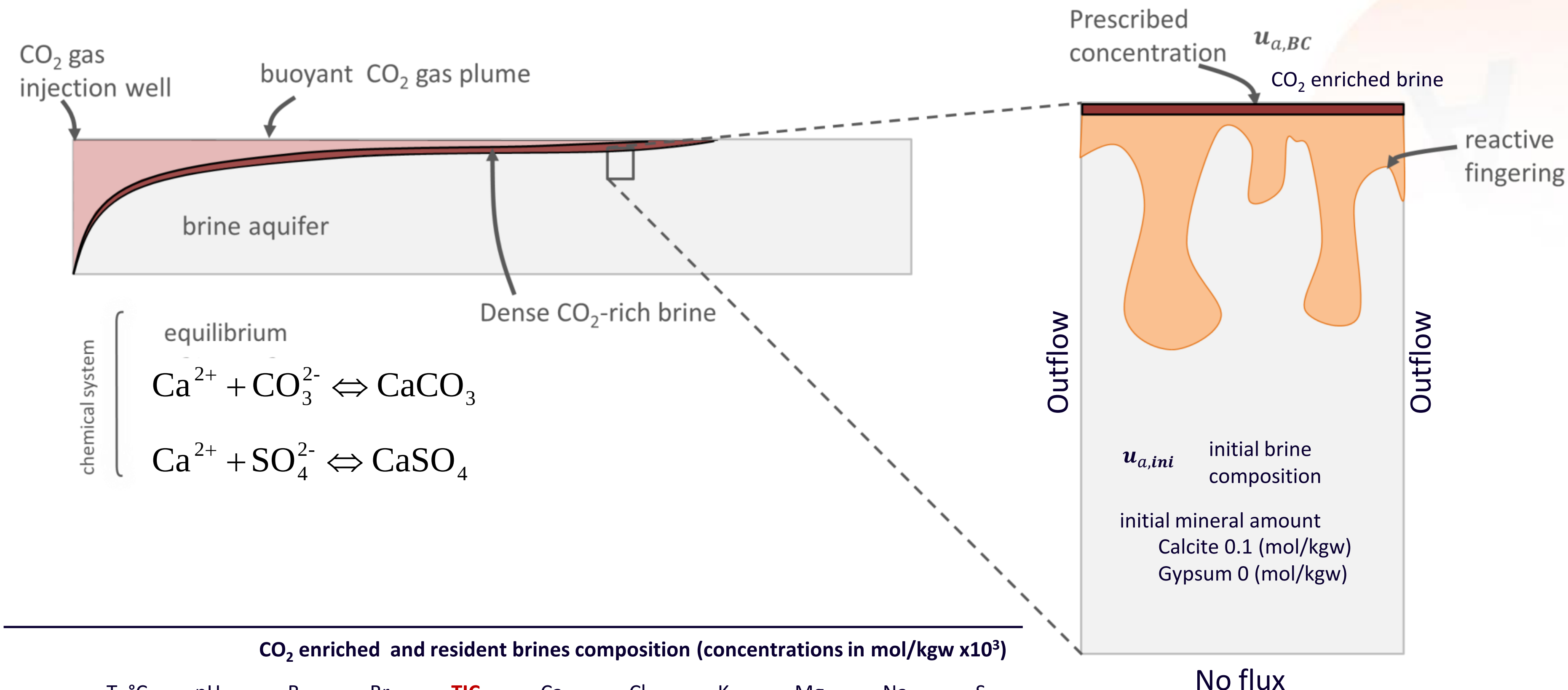




During injection CO_2 floats and extends through the top of the aquifer below the caprock. CO_2 dissolves into the resident brine increasing its density. This causes the brine to sink by means of fingering process. The resultant acid mixture reacts with the rock, leading to CO_2 precipitation as carbonate.

Objective and conceptual model

Study the interaction between convective mixing and reactive transport processes related to CO_2 dissolution into the resident brine of a carbonated aquifer.



chemical system

equilibrium

$$Ca^{2+} + CO_3^{2-} \Leftrightarrow CaCO_3$$

$$Ca^{2+} + SO_4^{2-} \Leftrightarrow CaSO_4$$

CO_2 enriched and resident brines composition (concentrations in mol/kgw x10^3)

	T, °C	pH	B	Br	TIC	Ca	Cl	K	Mg	Na	S
$u_{a,BC}$	25	3.261	1.465	1.036	1443	53.51	593.6	14.34	26.26	470.7	24.31
$u_{a,ini}$	25	6.980	1.465	1.036	1.370	53.51	593.6	14.34	26.26	470.7	24.31

Methodology

1. Governing equations

Flow in porous media

$$\frac{\partial(\phi\rho_l)}{\partial t} = \nabla \cdot \rho_l \boldsymbol{q}_l$$

The coupled system of equations is solved using the widely spread Sequential Non Iterative Approach (SNIA), which is based on the Operator Splitting concept.

Reactive transport

$$\boldsymbol{U}_a \frac{\partial(\phi\rho_l \boldsymbol{c}_a)}{\partial t} + \boldsymbol{U}_d \frac{\partial(\phi\rho_l \boldsymbol{c}_d)}{\partial t} + \boldsymbol{U}_m \frac{\partial((1-\phi)\rho_m \boldsymbol{c}_m)}{\partial t} = \boldsymbol{U}_a L_l(\boldsymbol{c}_a) + \boldsymbol{U}\boldsymbol{S}_k{}^{t} \boldsymbol{r}_m(\boldsymbol{c})$$

Density dependent on temperature and composition

$$\rho_l = \rho_l(\boldsymbol{c}_a, T)$$

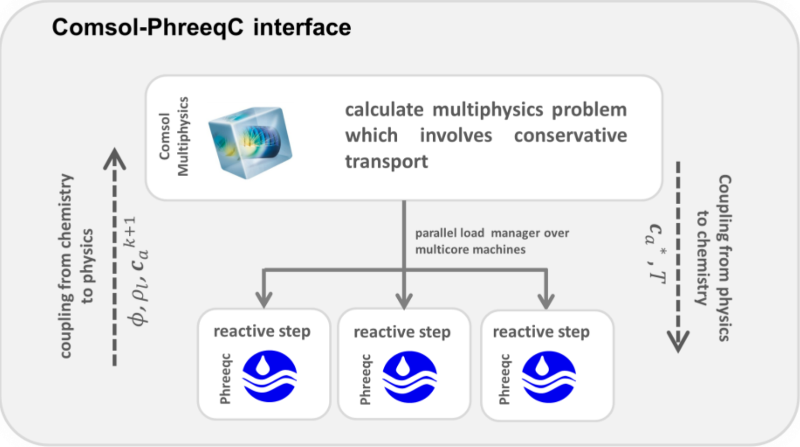
Porosity and permeability updated from mineral precipitation

$$\phi^{k+1} = \phi^k + \omega_l^{w} \sum_{m=1}^{N_m} V_m \, c_m^{k+1}$$

$$\boldsymbol{\kappa} = \boldsymbol{\kappa}_0 \left(\frac{\phi}{\phi_0}\right)^3$$

2. Numerical tool

The interface Comsol-PhreeqC (iCP) was used to perform the simulations. iCP combines the key capabilities of PhreeqC and Comsol in a single reactive transport simulator.



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Interface Comsol-PhreeqC (iCP)

Comsol Multiphysics v4.3

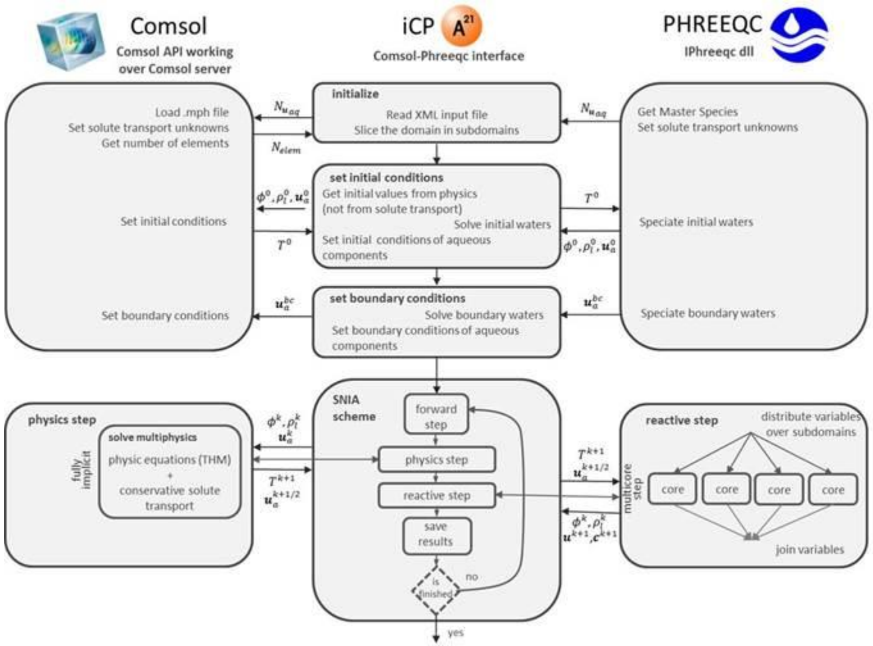
Code that allows simulating different physical phenomena based on differential equations using finite element methods.

PhreeqC v2

Code to simulate **chemical reactions** and transport processes in aqueous systems.

iCP

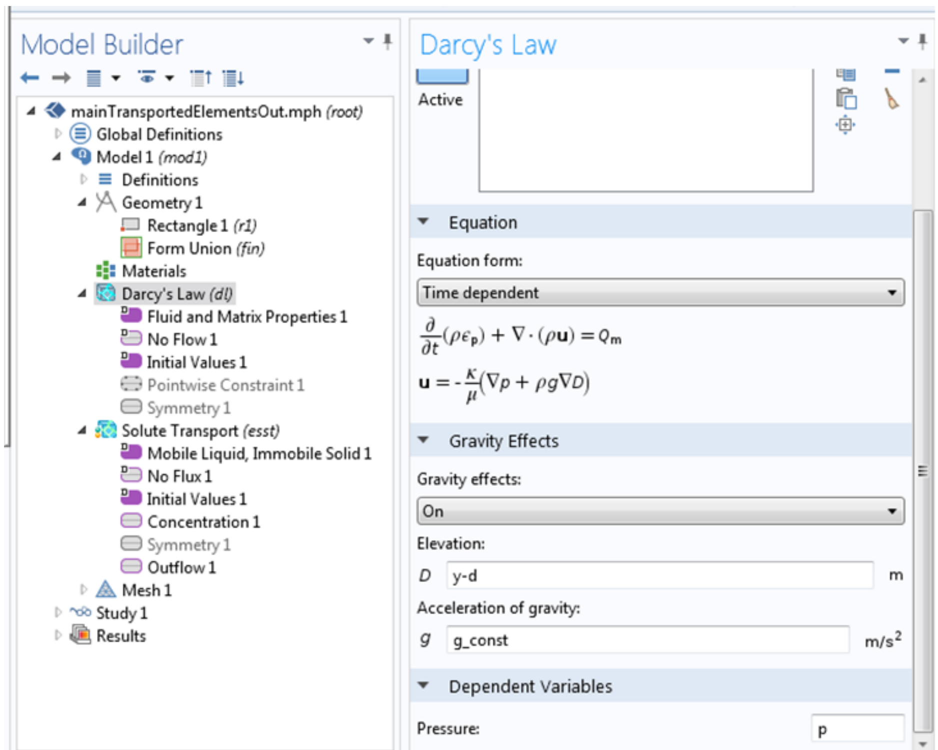
Interface developed at Amphos 21 that couple PhreeqC to Comsol, thus allowing to simulate a wide range of **reactive transport** problems in hydrogeochemistry, hydrology, mining, etc.



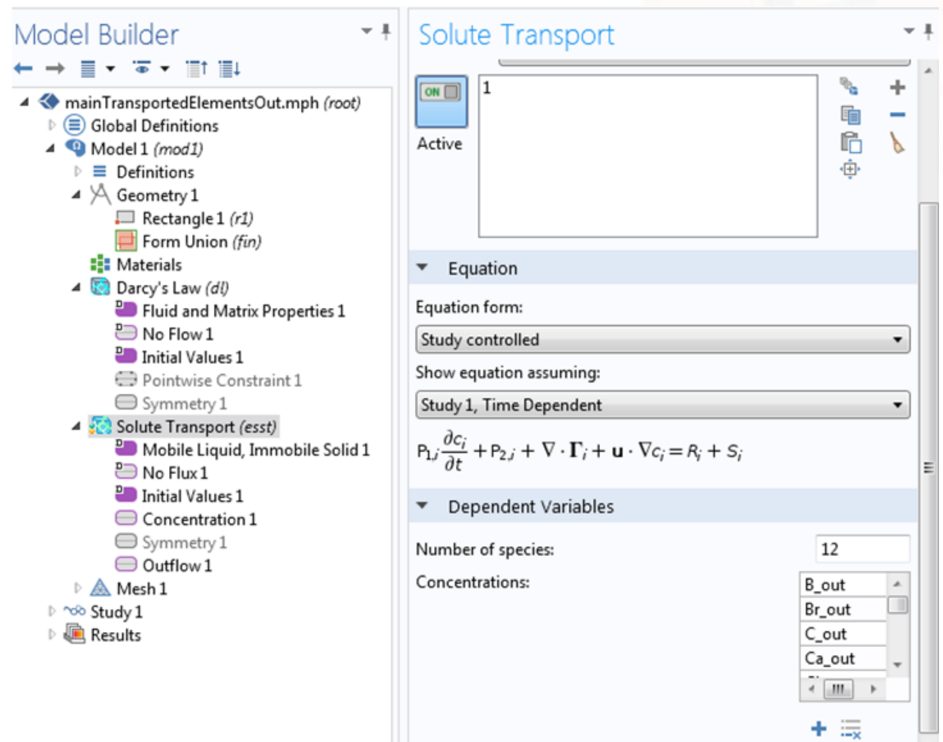
Used Comsol characteristics

The model was implemented using the Darcy's Law (Subsurface Flow module, Fluid Flow), and Solute Transport (Chemical Species Transport module) physics.

Darcy's Law



Solute transport



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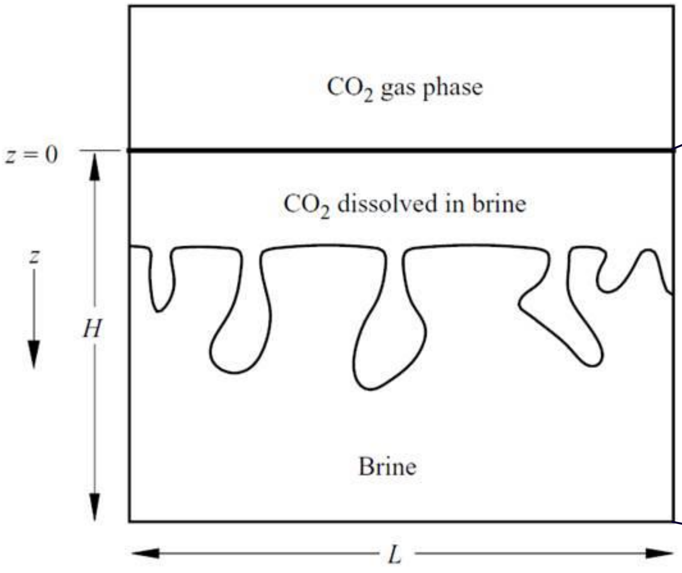
Onset of convection during CO_2 injection: Single-phase flow with reactive transport. *Fingering effects*

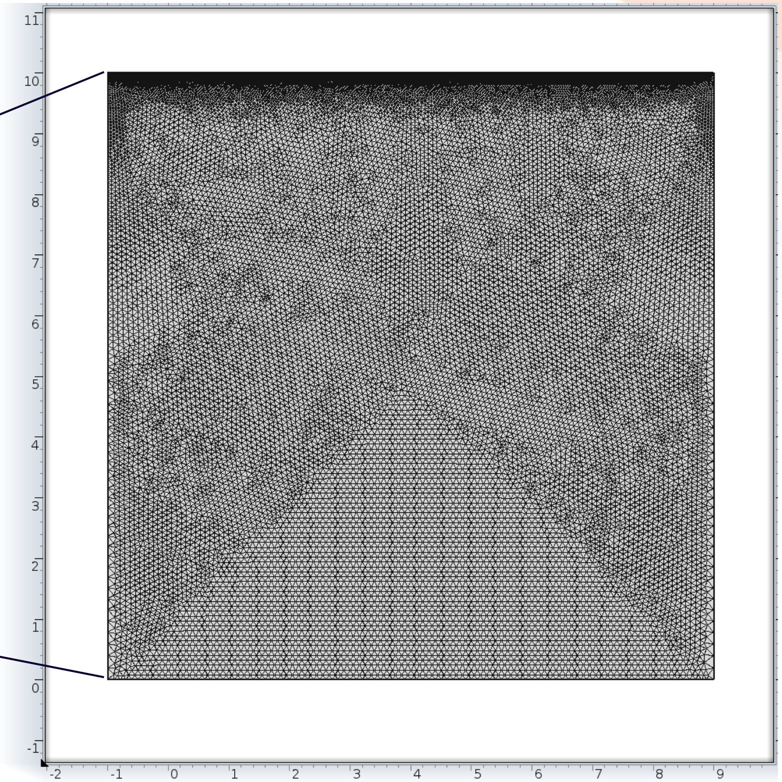
Conceptualization

Riaz et al., 2006. *J. Fluid Mech.*, vol 548, pp. 87-111



t_{ini}, s	t_{end}, s	Nº time steps
0	$3x10^6$	1
$3x10^6$	10^7	9
10^7	10^8	99
10^8	$3x10^8$	200

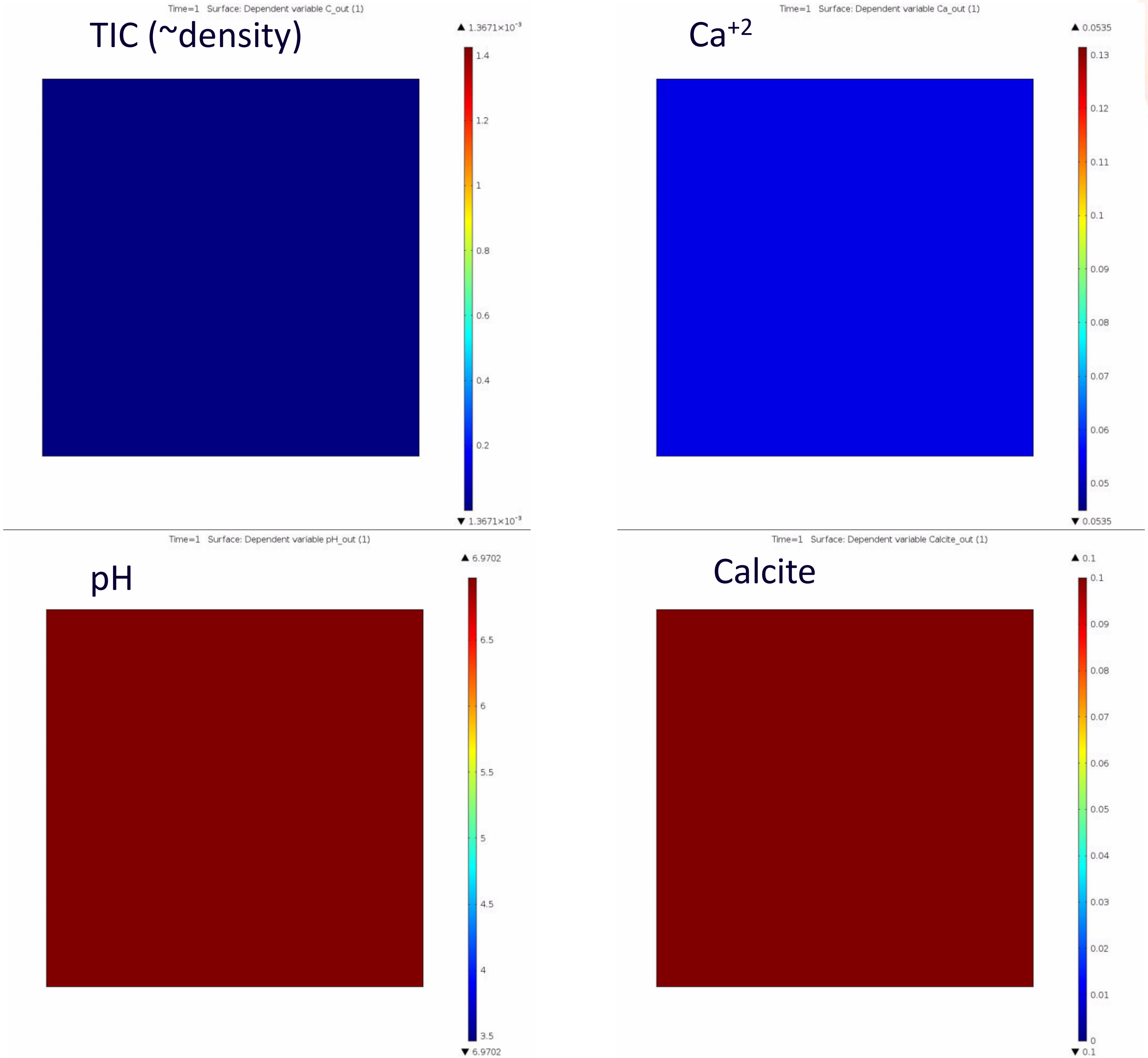
Comsol simulation



41572 triangular elements

Simulation time 9.5 years ($3x10^8$ s)

Fingering effects: impact on mineral dissolution



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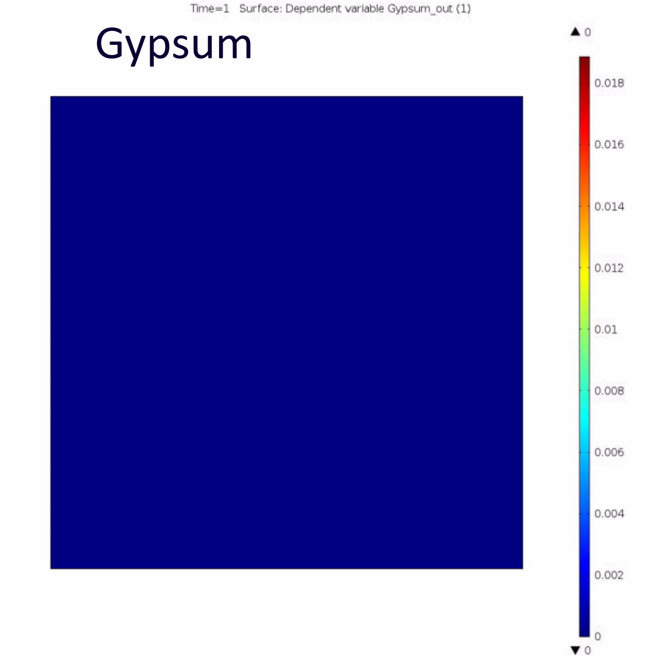
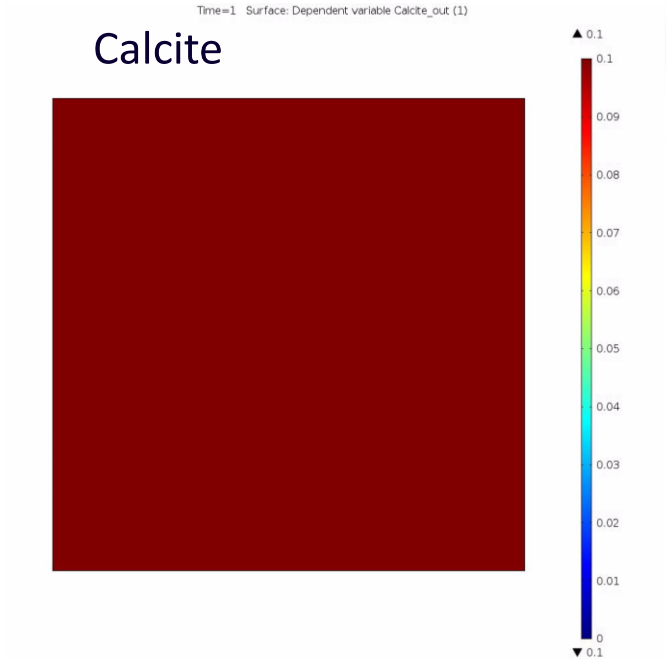
Mineral precipitation/dissolution and porosity changes

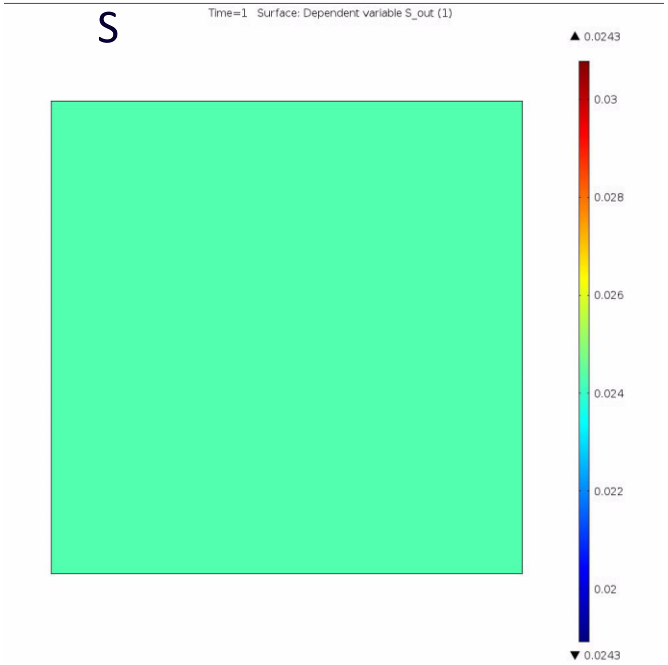
Gypsum



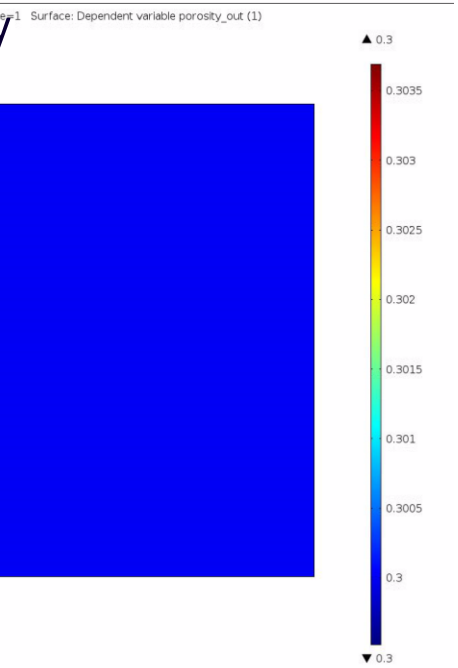
Calcite



S



Porosity



Conclusions

- Physical instability results in fingering of brine rich in CO_2.

- Fingering of acidic CO_2-rich brine can lead to:
  - Heterogeneous distributions of Ca^{2+} and SO_4^{2-}
  - Non-uniform calcite dissolution and gypsum precipitation patterns.

- Flow and reactive transport are strongly coupled: porosity and permeability are significantly affected by dissolution/precipitation patterns; fingering enhances mixing and promotes chemical reactions.

- The interface iCP (Comsol-PhreeqC) is a powerful tool to evaluate mineralization and dissolution changes that occur during CO_2 injection and storage.

Acknowledgements

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SEVENTH FRAMEWORK PROGRAMME

carbfix

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