Efficient and robust open-source modelling platform for Energy Transition applications

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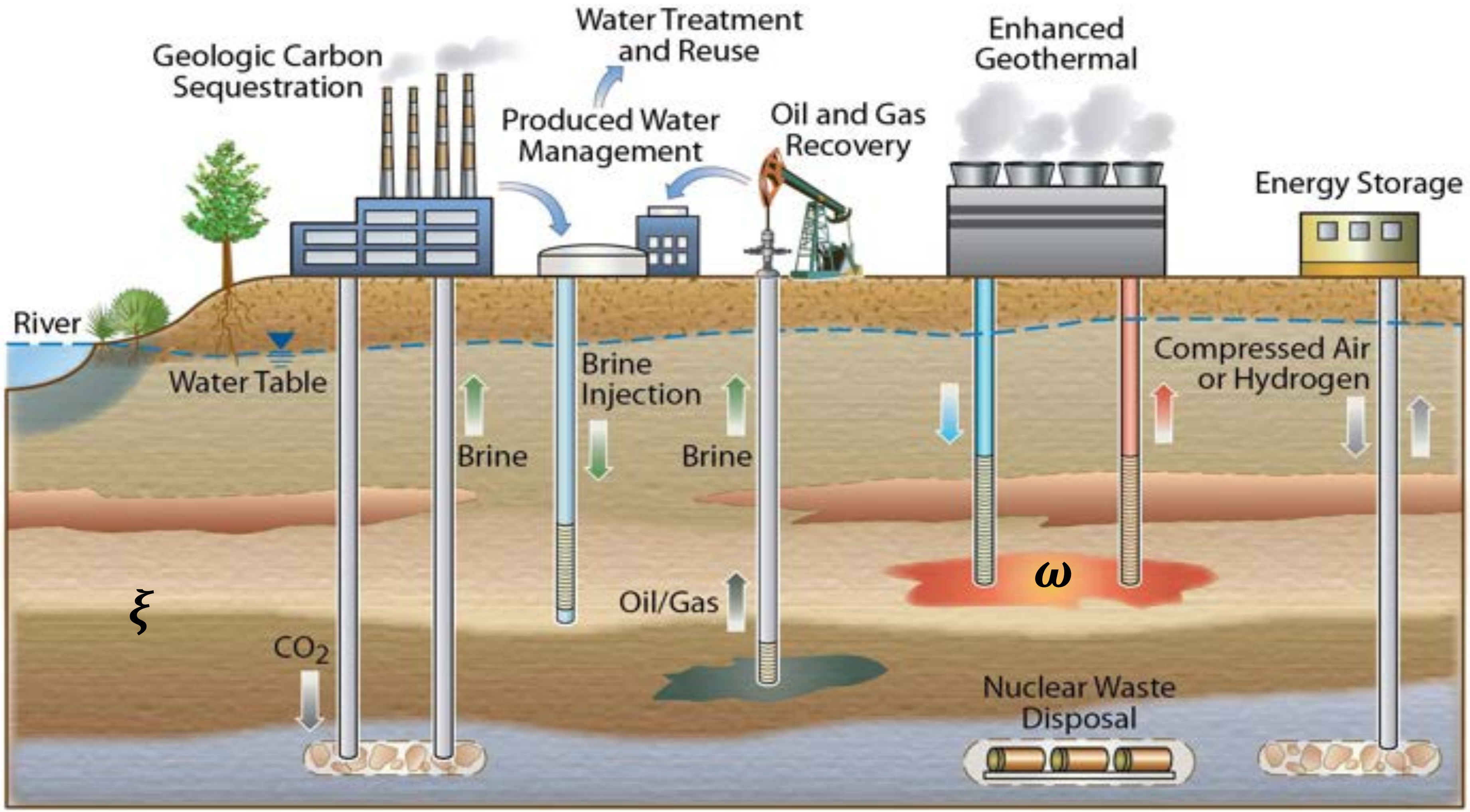
Modelling of energy transition problems

- Reservoir simulation is an important tool for an integration of different information from various sources and scales
- To describe industrial applications relevant to energy transition, we need to employ complex formulation of **multiphase** flow and **thermal-compositional reactive** transport in porous media
- Strong heterogeneities in subsurface properties demand uncertainty analysis with **ensembles** of simulation models

The robust and efficient reservoir simulation capabilities are wanted!

Multiphase thermal-compositional formulation

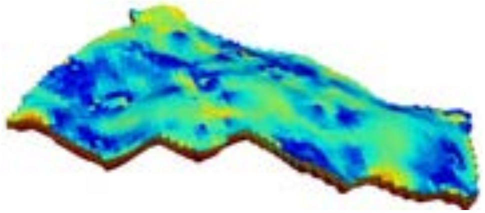


Source: LBNL

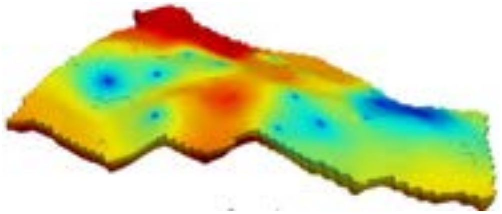
PDE for Energy Transition applications

$$\boldsymbol{g}(\boldsymbol{\omega}) = \boldsymbol{a}_t(\boldsymbol{\omega}, \boldsymbol{\xi}) + \nabla \cdot \boldsymbol{b}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \Delta \boldsymbol{c}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \boldsymbol{d}(\boldsymbol{\omega}, \boldsymbol{\xi}) = 0$$

$\boldsymbol{\xi} = \{\boldsymbol{G}, \boldsymbol{\phi}, \boldsymbol{K}\}$



$\boldsymbol{\omega} = \{\boldsymbol{p}, \boldsymbol{T}, \boldsymbol{z}\}$



Compressibility, phase change and convection

$$\boldsymbol{g}(\boldsymbol{\omega}) = \frac{\phi_0 V}{\Delta t}[\boldsymbol{\alpha}(\boldsymbol{\omega}) - \boldsymbol{\alpha}(\boldsymbol{\omega}_n)] + \sum_l v_t^l \boldsymbol{\beta}\,(\boldsymbol{\omega}) = \mathbf{0}$$

$$\alpha_c(\boldsymbol{\omega}) = c(p)\ \sum_{j=1}^{n_p} x_{cj}\rho_j s_j,$$

$$\beta_c(\boldsymbol{\omega}) = \frac{1}{\Lambda}\sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l}$$

$$\boldsymbol{g}(\boldsymbol{\omega}) = \frac{\phi_0 V}{\Delta t}[\boldsymbol{\alpha}(\boldsymbol{\omega}) - \boldsymbol{\alpha}(\boldsymbol{\omega}_n)] + \sum_l v_t^l \boldsymbol{\beta}(\boldsymbol{\omega}) + \sum_l \mathbf{D}^l(\boldsymbol{\chi}^l - \boldsymbol{\chi})\boldsymbol{\gamma}(\boldsymbol{\omega}) + \mathrm{V}\boldsymbol{\delta}(\boldsymbol{\omega}) = \mathbf{0}$$

+ diffusion and reactions

$$\gamma_c(\boldsymbol{\omega}) = c(p)\sum_{j=1}^{n_p} x_{cj}\rho_j s_j d_{cj}, \qquad \delta_c(\boldsymbol{\omega}) = \sum_{\mathrm{k}=1}^{n_k} \nu_{ck} r_k$$

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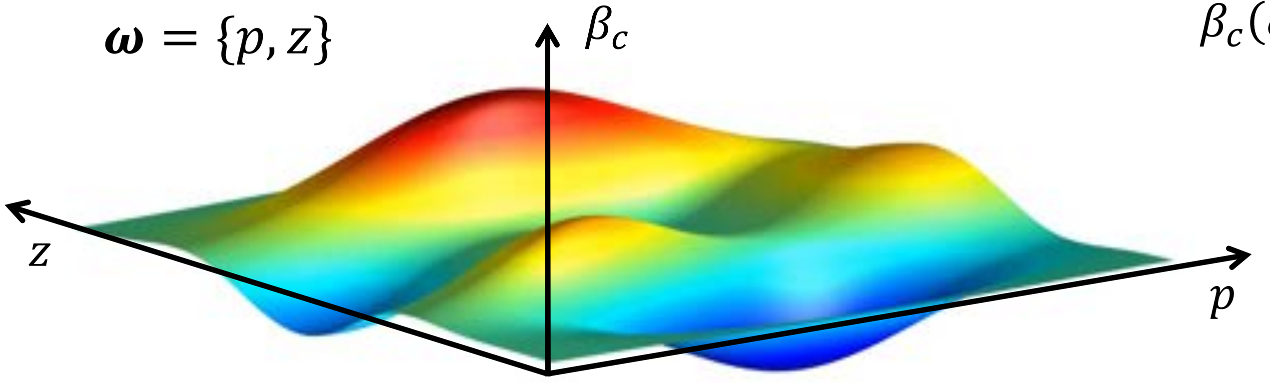
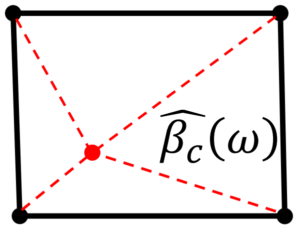
Operator-Based Linearization

$$\boldsymbol{\omega} = \{p, z\}$$



$$\beta_c(\boldsymbol{\omega}^1) = \frac{1}{\Lambda}\sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l} \qquad \beta_c(\boldsymbol{\omega}^2) = \frac{1}{\Lambda}\sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l}$$



$$\beta_c(\boldsymbol{\omega}^3) = \frac{1}{\Lambda}\sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l} \qquad \beta_c(\boldsymbol{\omega}^4) = \frac{1}{\Lambda}\sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l}$$

$$\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{\omega}} = \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{\omega}} \bar{\boldsymbol{a}}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \frac{\partial \boldsymbol{\beta}}{\partial \boldsymbol{\omega}} \bar{\boldsymbol{b}}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \frac{\partial \boldsymbol{\gamma}}{\partial \boldsymbol{\omega}} \bar{\boldsymbol{c}}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \frac{\partial \boldsymbol{\delta}}{\partial \boldsymbol{\omega}} \bar{\boldsymbol{d}}(\boldsymbol{\omega}, \boldsymbol{\xi}) + \bar{\boldsymbol{f}}(\boldsymbol{\omega}, \boldsymbol{\xi})$$

$$\left|\widehat{\beta_c} - \beta_c\right| \le cA^2 \sup_{\omega} |\nabla^2 \beta_c|$$

Voskov, JCP 2017

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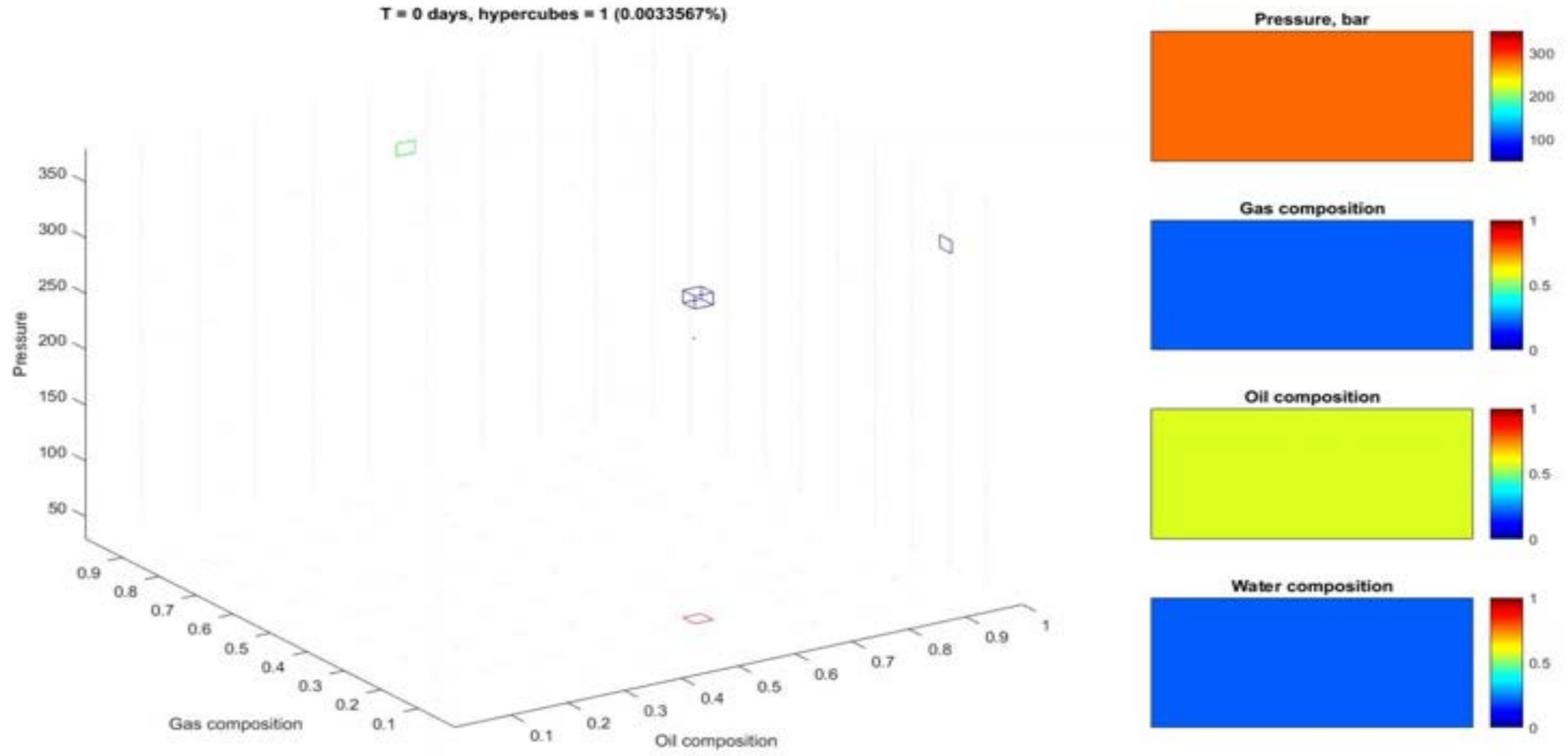
Adaptive parametrization



Khait and Voskov, JPSE, 2017

Generic thermal-compositional formulation

$$\frac{\partial}{\partial t}\int_{\Omega} M^c d\Omega + \int_{\Gamma} \boldsymbol{F}^c \cdot \boldsymbol{n} d\Gamma = \int_{\Omega} Q^c d\Omega$$

Mass conservation

$$M^c = \phi \sum_{j=1}^{n_p} x_{cj}\rho_j s_j \qquad c = 1, \ldots, n_c,$$

$$\boldsymbol{F}^c = \sum_{j=1}^{n_p} x_{cj}\rho_j \boldsymbol{u_j} + s_j \rho_j \mathbf{J}_{cj}, \quad c = 1, \ldots, n_c$$

$$Q^c = \sum_{k=1}^{n_k} v_{ck} r_k, \quad c = 1, \ldots, n_c$$

Energy conservation

$$M^{n_c+1} = \phi \sum_{j=1}^{n_p} \rho_j s_j U_j + (1-\phi) U_r$$

$$\boldsymbol{F}^{n_c+1} = \sum_{j=1}^{n_p} h_j \rho_j \boldsymbol{u_j} + \kappa \nabla T$$

$$Q^{n_c+1} = \sum_{k=1}^{n_k} v_{ek} r_{ek}$$

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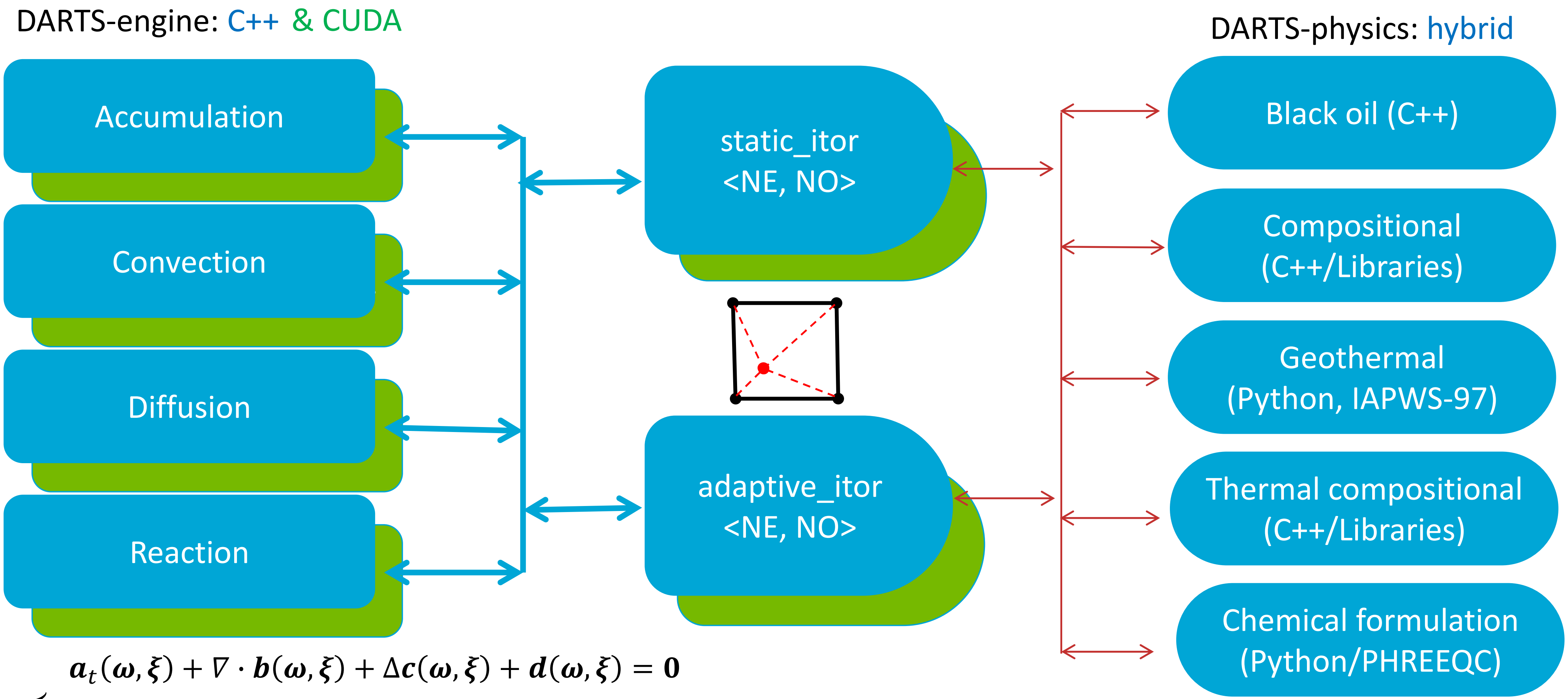
Delft Advanced Research Terra Simulator



$$\boldsymbol{a}_t(\boldsymbol{\omega},\boldsymbol{\xi}) + \nabla \cdot \boldsymbol{b}(\boldsymbol{\omega},\boldsymbol{\xi}) + \Delta \boldsymbol{c}(\boldsymbol{\omega},\boldsymbol{\xi}) + \boldsymbol{d}(\boldsymbol{\omega},\boldsymbol{\xi}) = \boldsymbol{0}$$

$$\boldsymbol{\alpha}(\boldsymbol{\omega}), \boldsymbol{\beta}(\boldsymbol{\omega}), \boldsymbol{\gamma}(\boldsymbol{\omega}), \boldsymbol{\delta}(\boldsymbol{\omega}), \ldots$$

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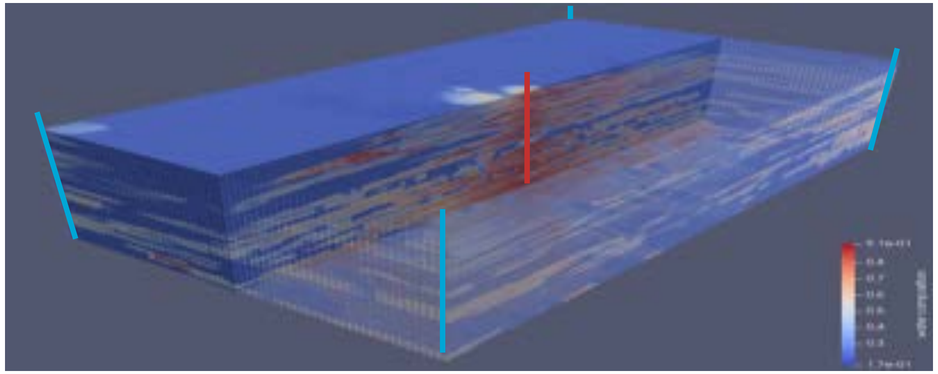
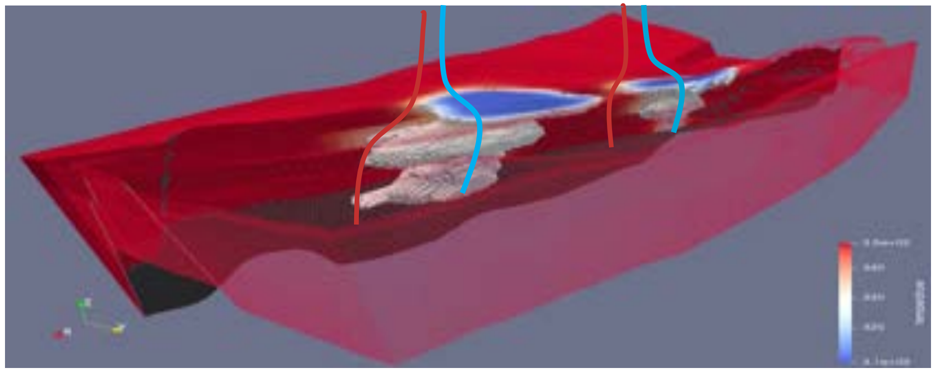
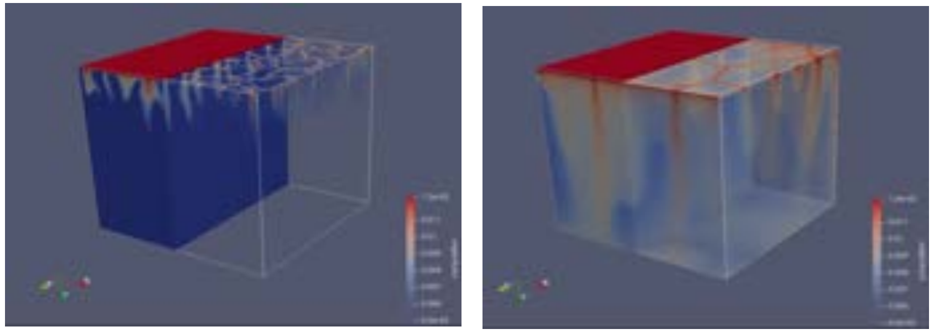
Delft Advanced Research Terra Simulator

- CO_2 injection for EOR
  - 1.1M active blocks, 5.5 years
  - 4 unknowns per block
  - CPU*: 20 min, GPU: 3.5 min
- Geothermal model
  - 3.2M active blocks, 100 years
  - 2 unknowns per block
  - CPU*: 49 min, GPU: 8 min
- CO_2 sequestration
  - 1.0M active blocks, 3000 years
  - 2 unknowns per block
  - CPU*: 3.8 hours, GPU: 55 min







*OpenMP on 20 physical cores

Khait and Voskov, SPE, 2021; Lyu et al., IJGGC, 2021; Wang et al., 2021

Thermodynamic model for CO_2-gas-brine-oil systems

- Gas component model: ignore effects of water component presence in gas phase

$$f_i^g = p\Phi_i y_i \qquad f_i^g = f_i^l \qquad f_i^l = h_i \gamma_i x_i$$

Henry constants

Peng-Robinson Equation of State

$$K_i = \frac{y_i}{x_i} = \frac{h_i \gamma_i}{p\Phi_i}$$

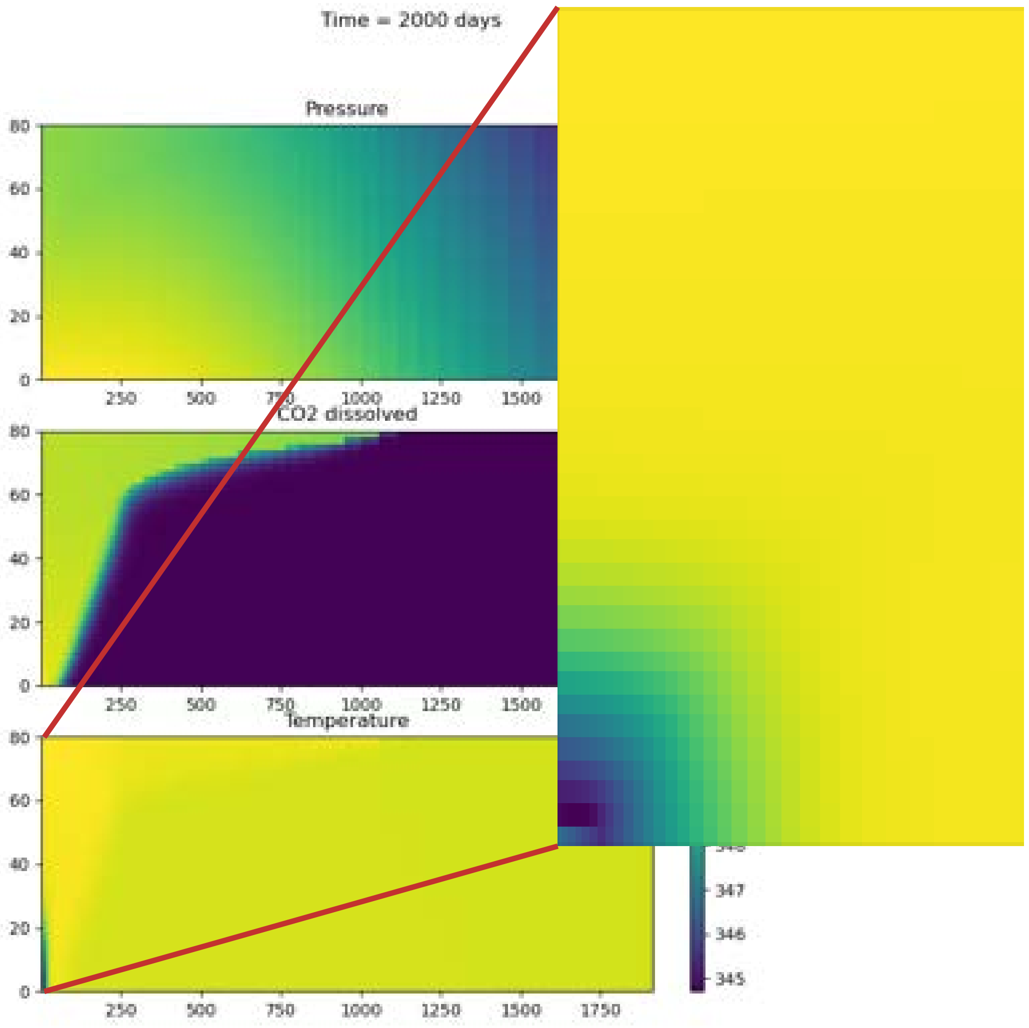
Activity model

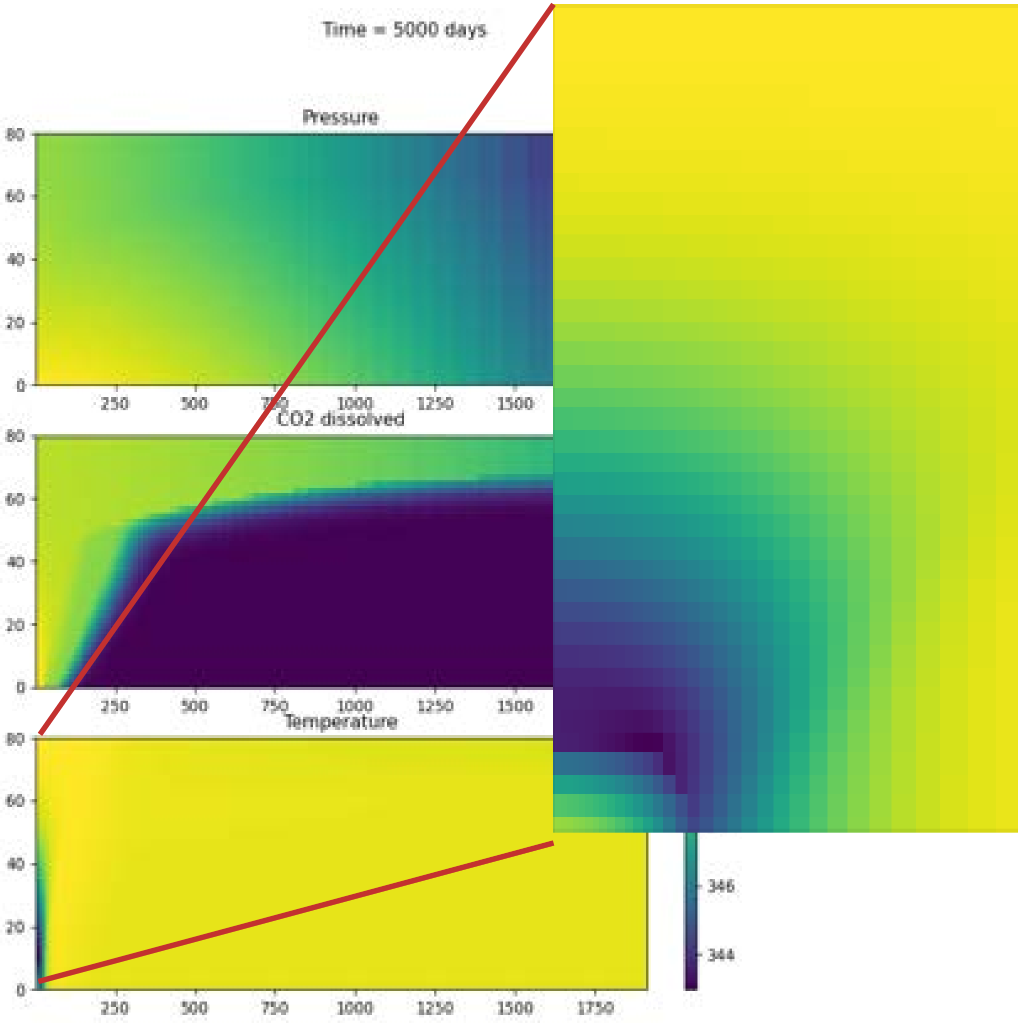
- Water component model: activity of water can be approximated by its mole fraction in liquid phase

$$K_{H_2O} = \frac{y_{H_2O}}{x_{H_2O}} = \frac{K^0_{H_2O}}{\Phi_{H_2O}p} exp\left[\frac{(p-1)V_{H_2O}}{RT}\right]$$

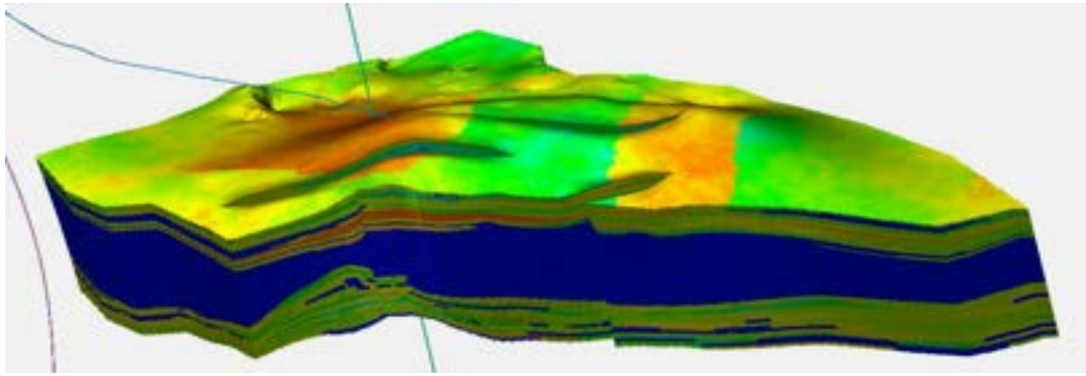
Morshuis, TU Delft, 2019

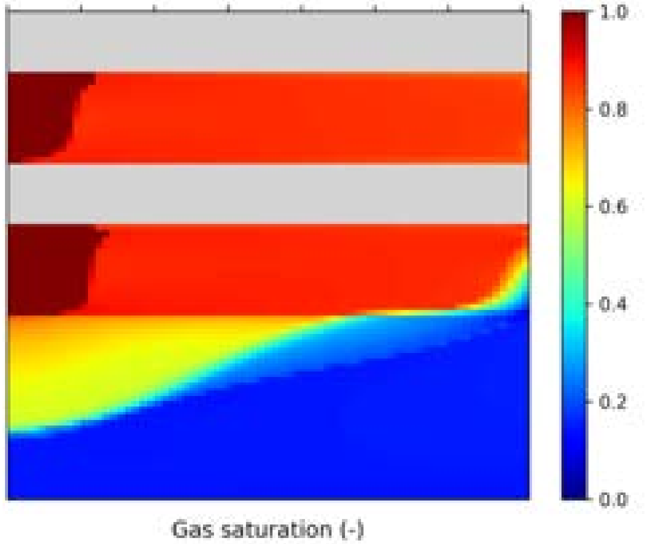
Joule-Thomson cooling for mixture CO_2-C_1-brine

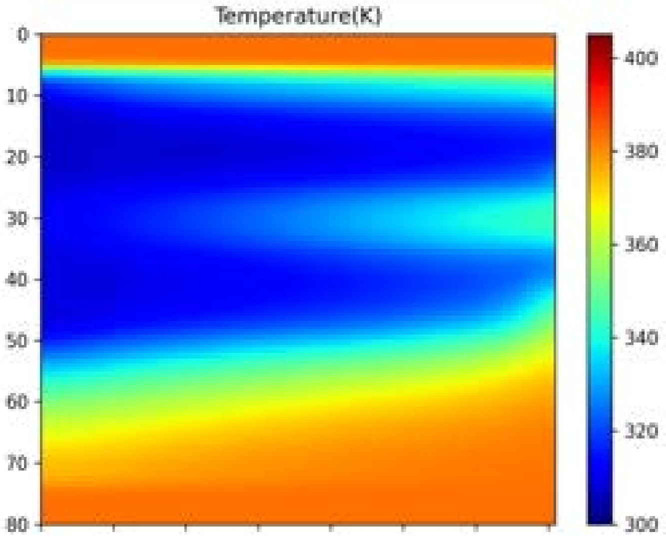


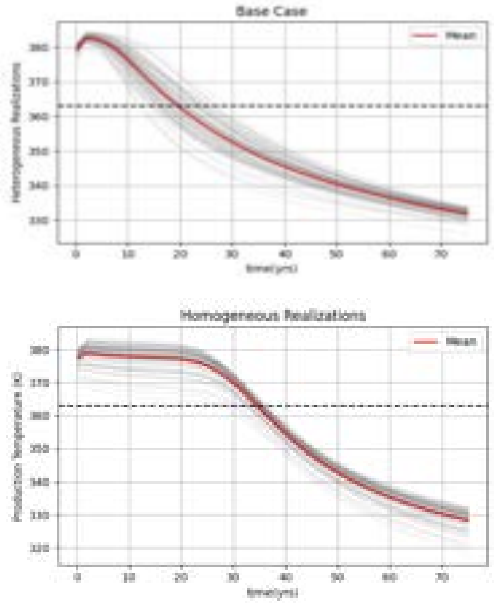


CO2 Plum Geothermal in depleted gas field









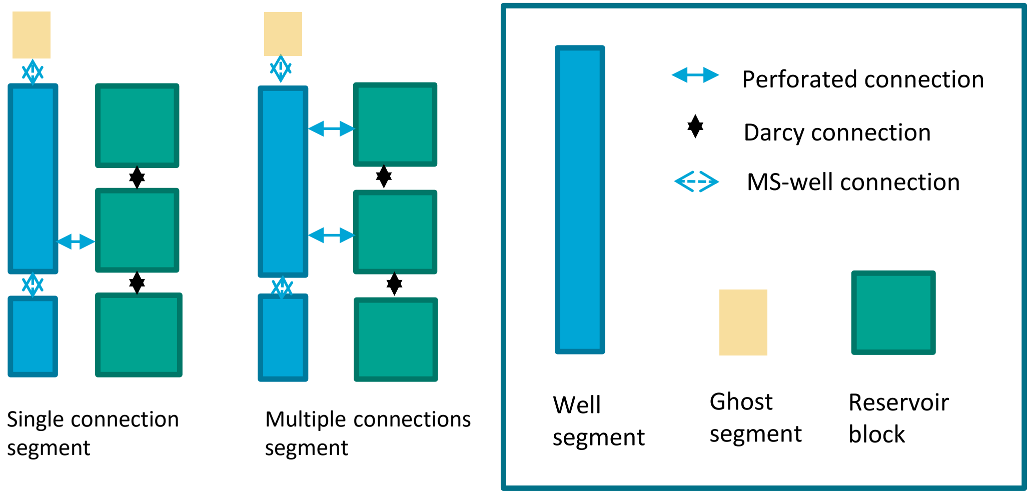
1st run ~ 2 hours, 2nd run ~ 20 minutes, … , 10th run ~ 5 minutes

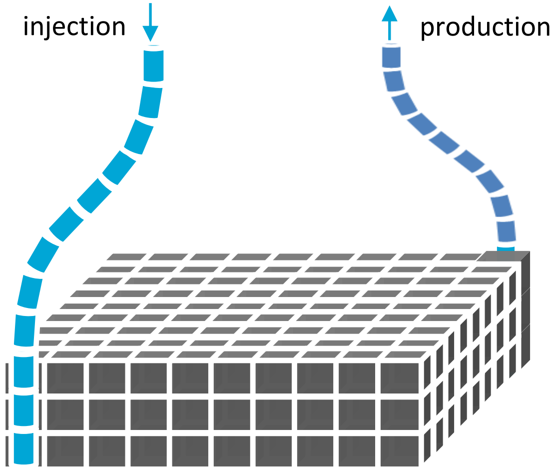
Multi-segmented well model

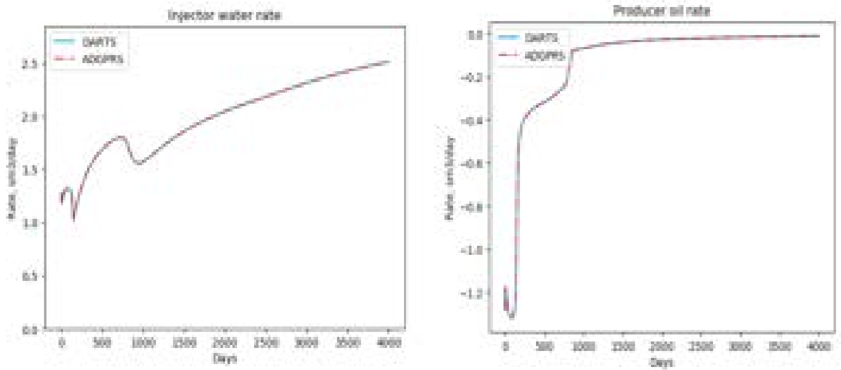
- Multi-physics in wellbore (thermal multiphase multi-component reactive flow and transport with heat loses)
- Complex well network (deviated, multilateral, annulus, etc.)

$$\frac{\phi_0 V}{\Delta t}\left[\boldsymbol{\alpha}(\boldsymbol{\omega}) - \boldsymbol{\alpha}(\boldsymbol{\omega}_n)\right] + \sum_l v_t^l(\boldsymbol{\xi},\boldsymbol{\omega})\boldsymbol{\beta}(\boldsymbol{\omega}) = \boldsymbol{g}(\boldsymbol{\omega})$$

$$\Delta p - \underbrace{\theta_h(\boldsymbol{\omega},\boldsymbol{\xi})}_{\text{Hydrostatic losses}} - \underbrace{\theta_f(\boldsymbol{\omega},\boldsymbol{\xi},v_t)}_{\text{Friction losses}} - \underbrace{\theta_a(\boldsymbol{\omega},\boldsymbol{\xi},v_t)}_{\text{Acceleration losses}} = \boldsymbol{g}^{\boldsymbol{w}}(\boldsymbol{\omega})$$

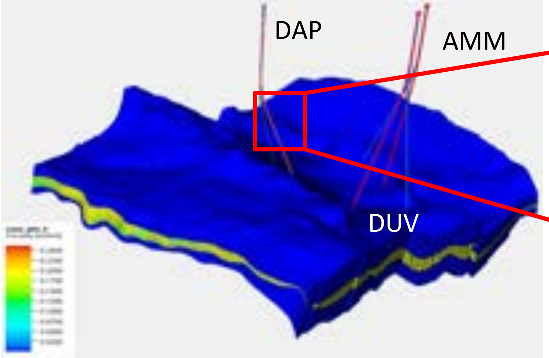




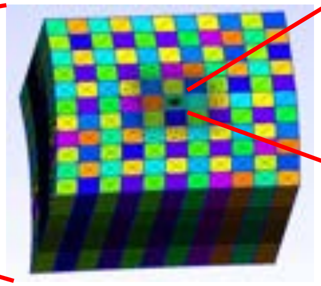


Near-well modeling

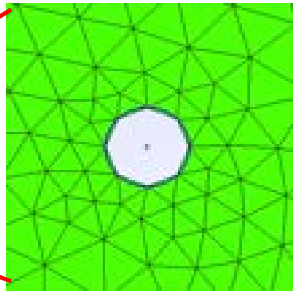
Petrel model



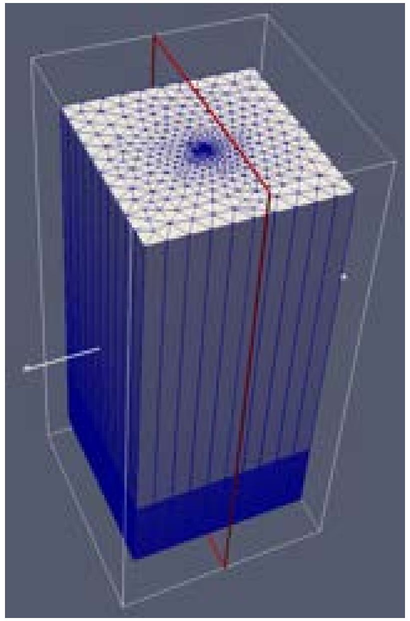
Gmsh model



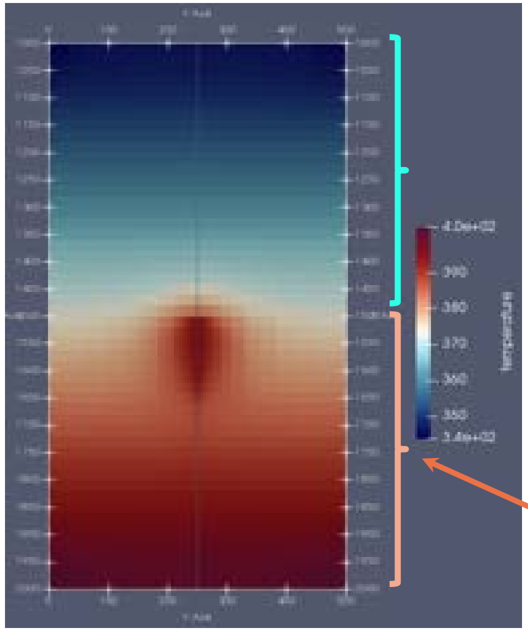
Well model



Wellbore discretization down to $r_w = 0.1\ m$

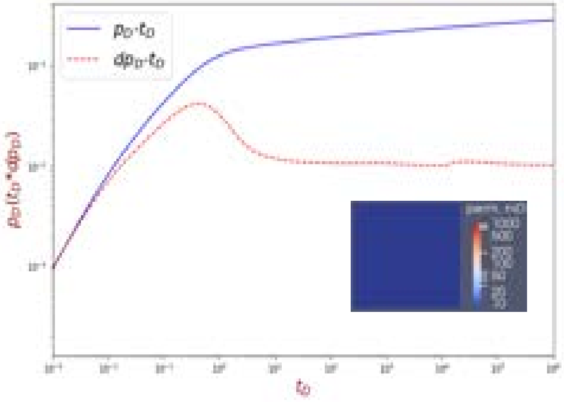


Effect of insulation

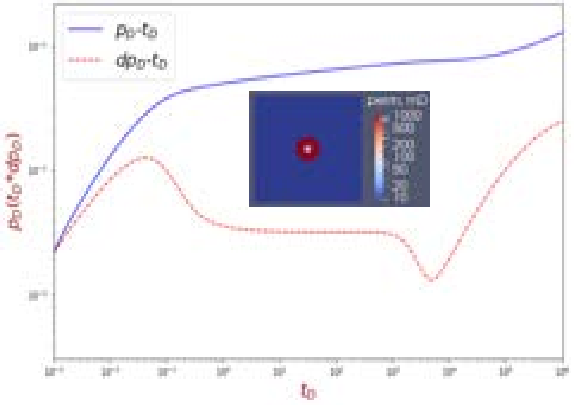


Non-insulated interval

Homogeneous



Heterogeneous



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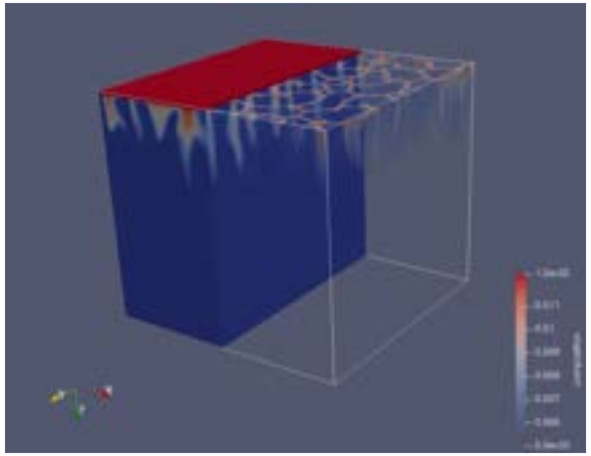
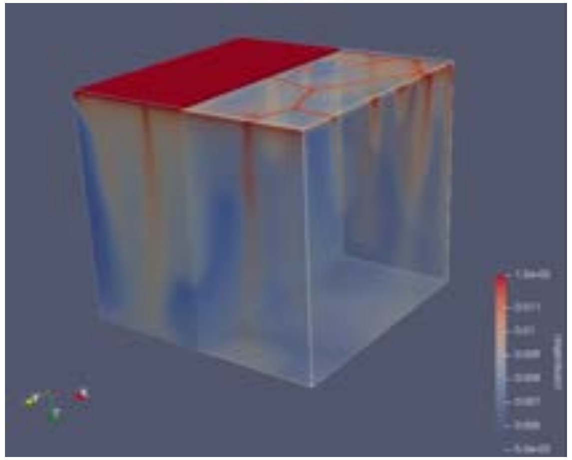
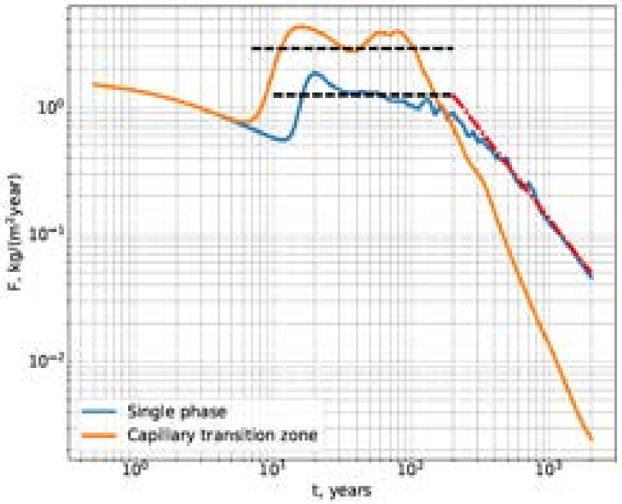
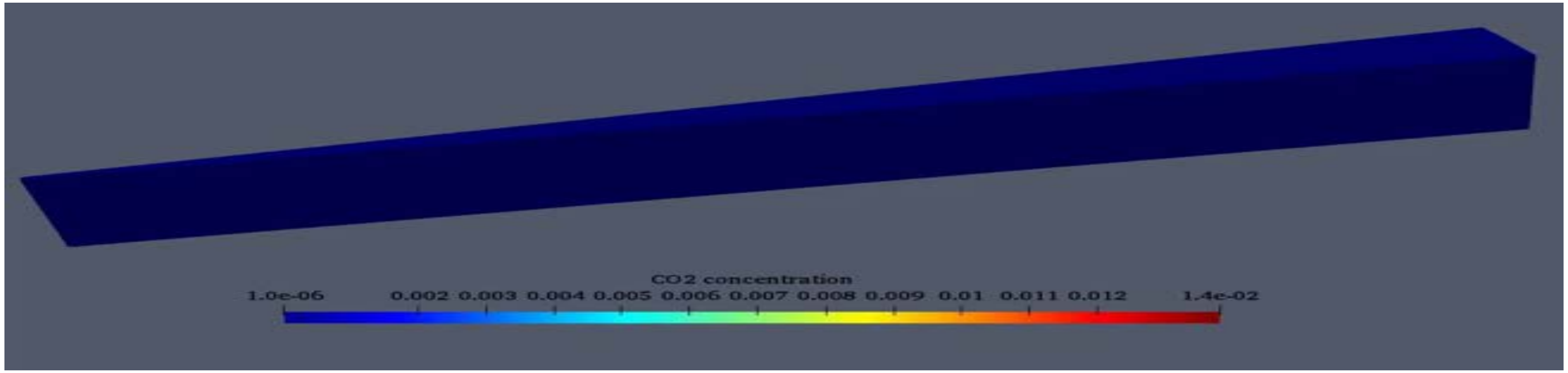
Enhanced CO_2 dissolution



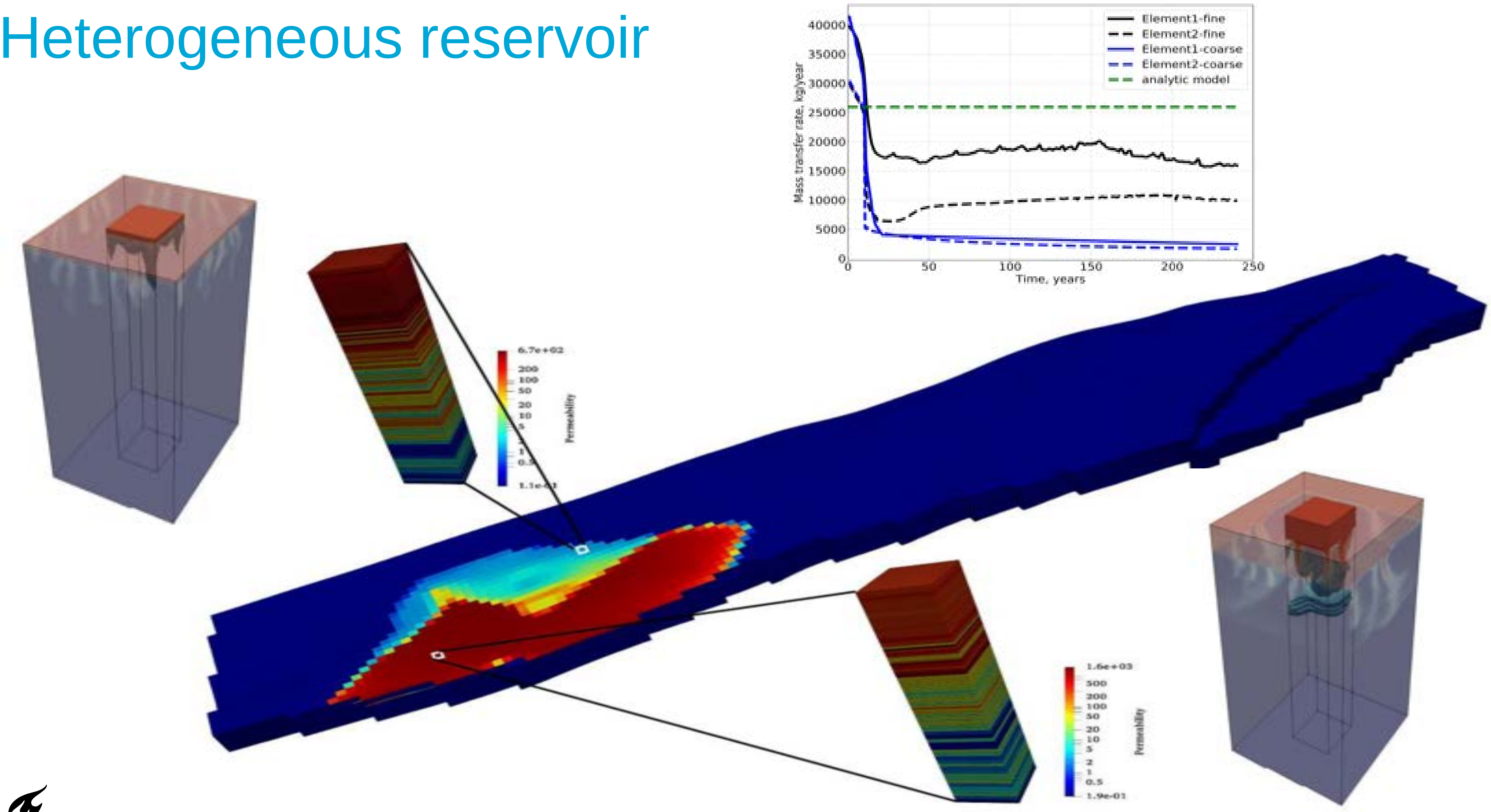






Lyu et al., IJGGC, 2021

Heterogeneous reservoir



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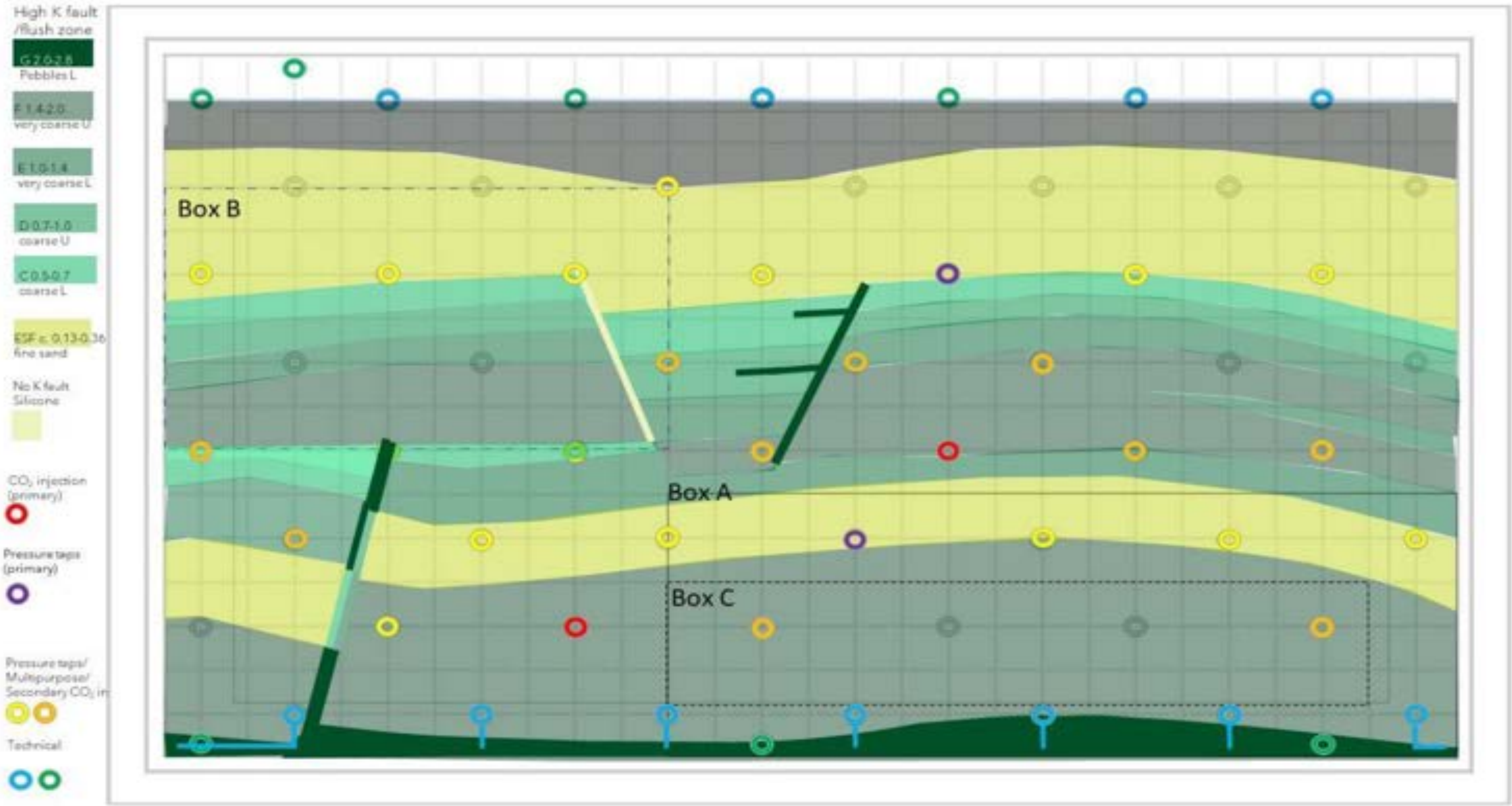
FluidFlower benchmark (University of Bergen)

Nordbotten et al., 2022

Model description



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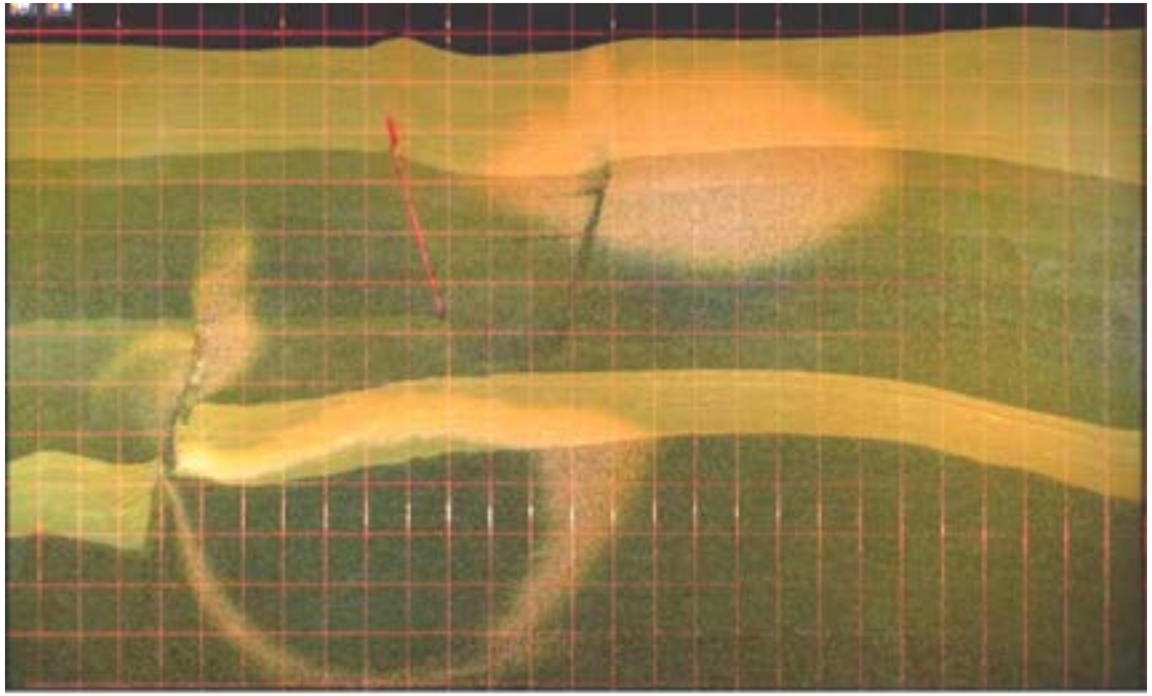
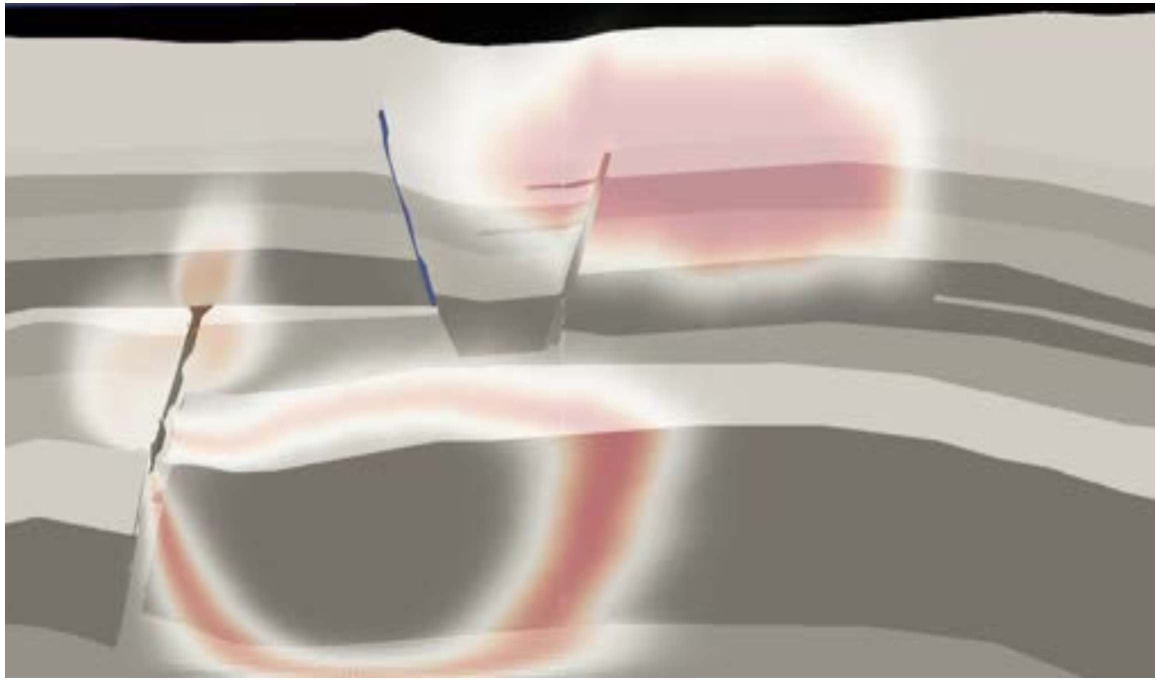
History matching using RML (single realization)

Tracer observations (high resolution images)

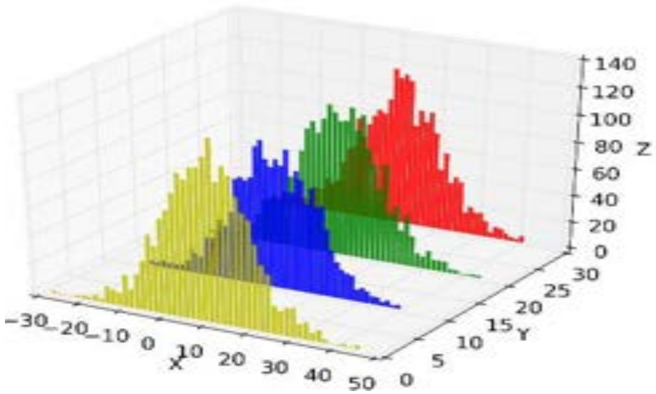


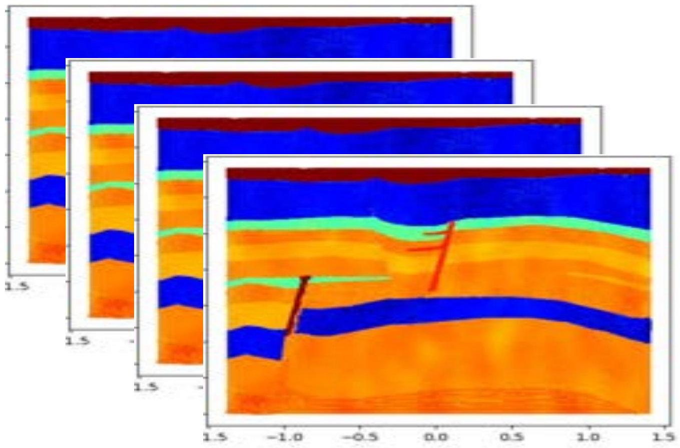
Inversed model (RML, 18278 forward runs for 100 priors)



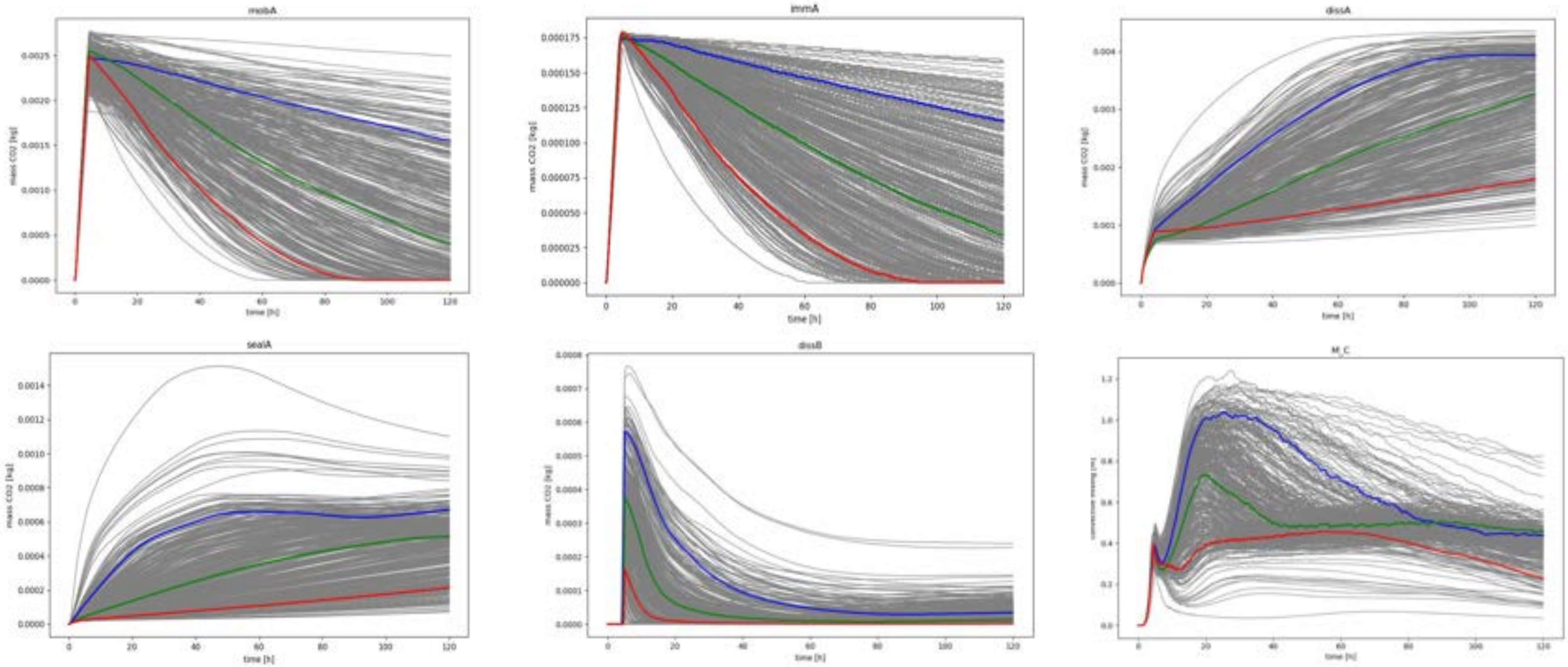
Uncertainty Quantification

- Temperature: $23°C \pm 2$, normal distribution
- Diffusion: $2 \cdot 10^{-10} - 2 \cdot 10^{-9}$, log-normal distribution
- Corey: base values with standard deviation from 5 to 50% for different parameters, normal distribution
- Models: 100 history matched permeability maps





UQ investigation (400 runs)



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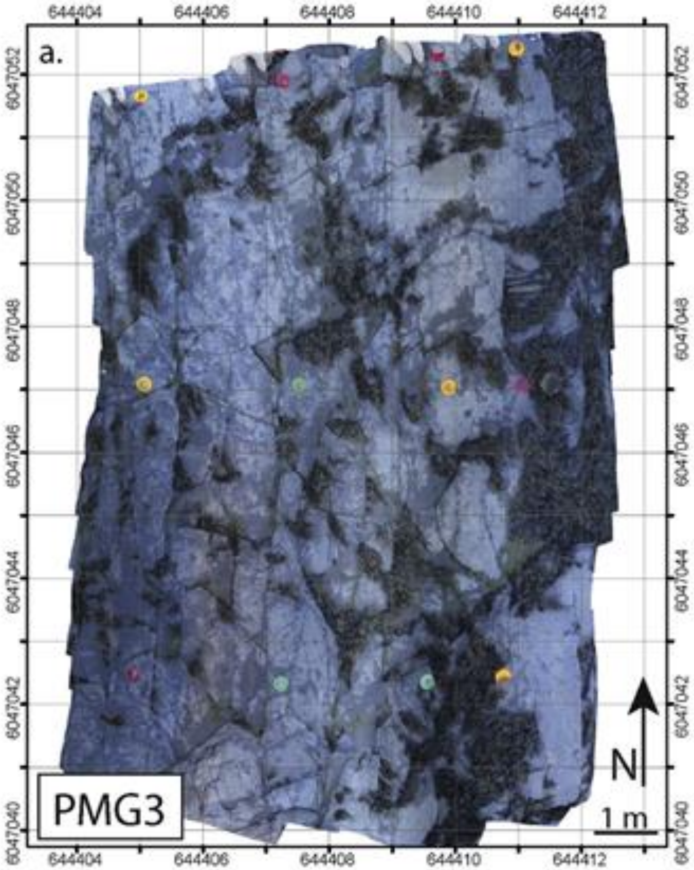
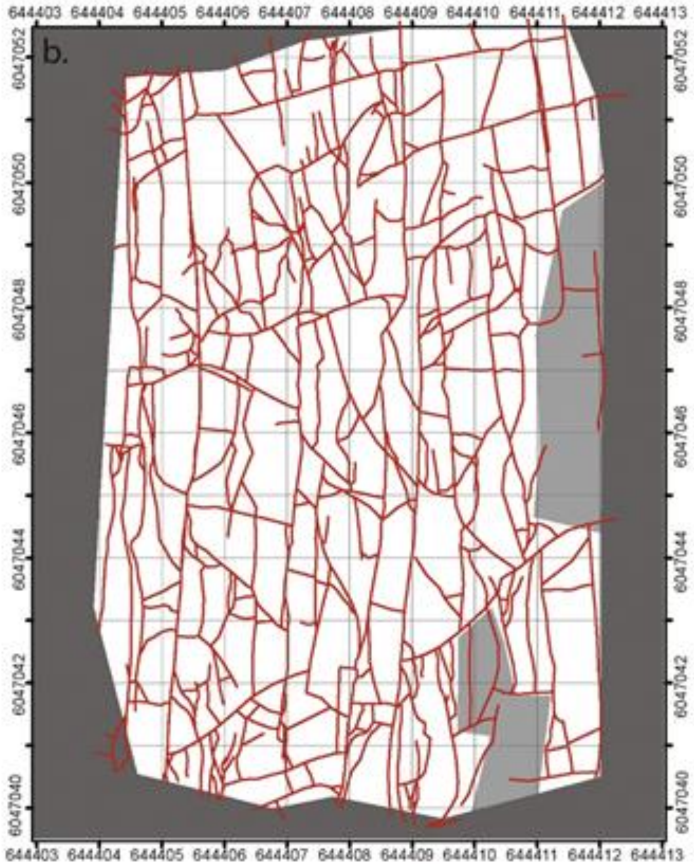
Modeling fractures

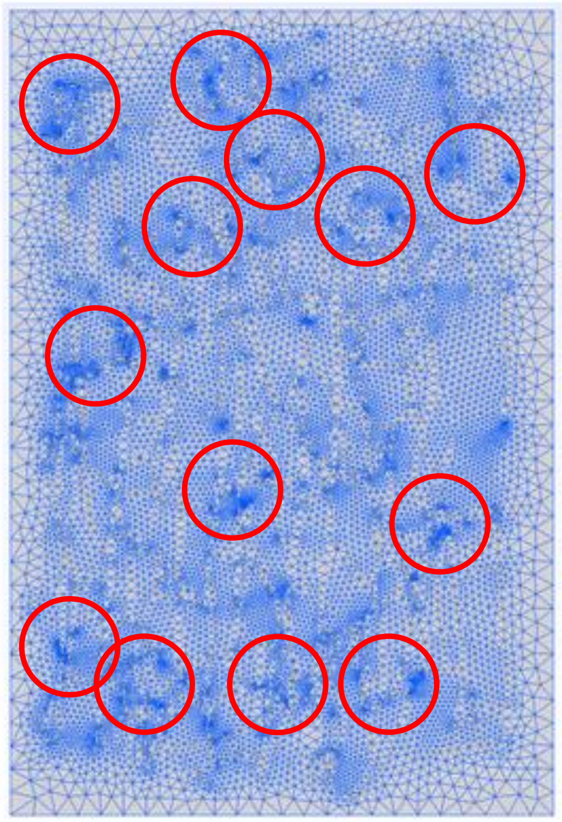


Acquire data



Interpret data

Problematic mesh!



Create numerical model (mesh)

Data from: Houben et al., 2017; Boersma et al., 2019

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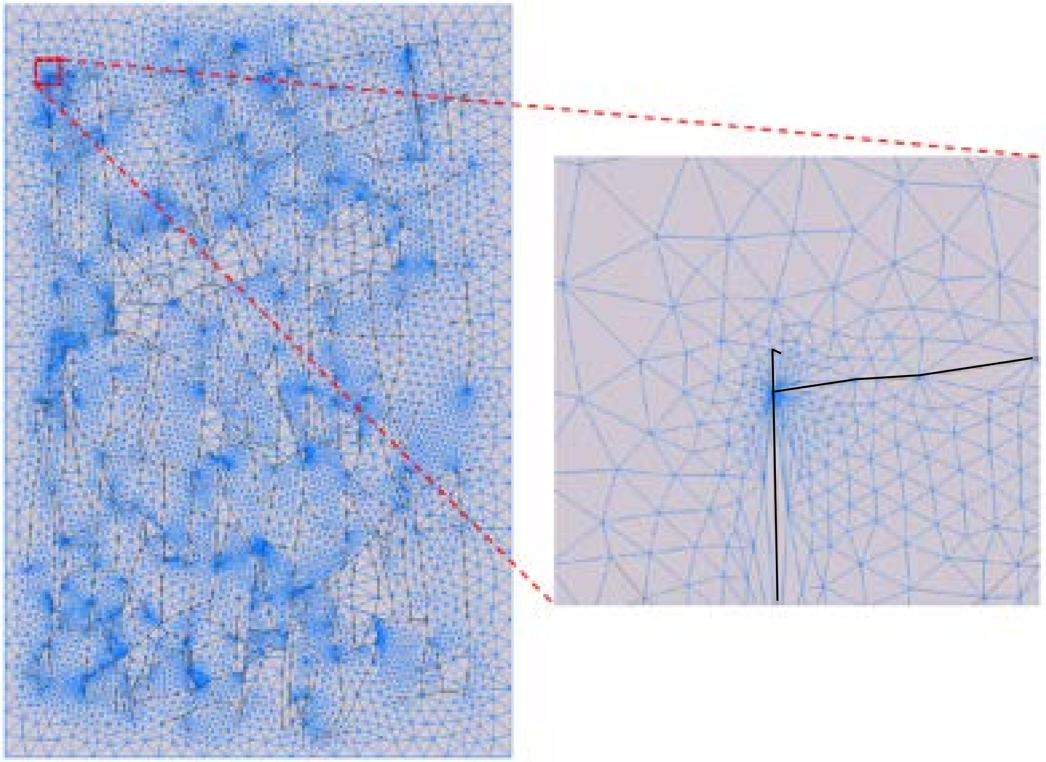
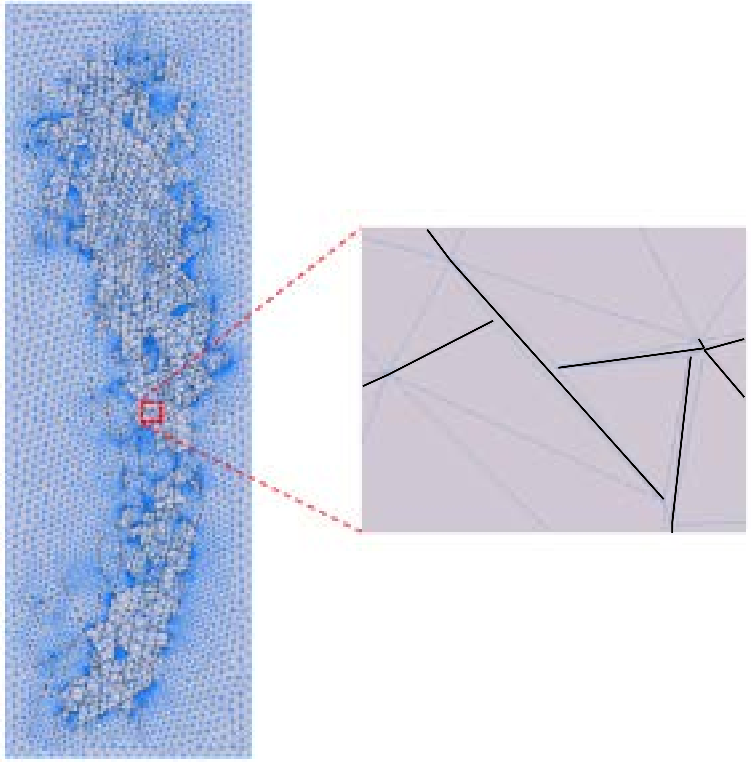
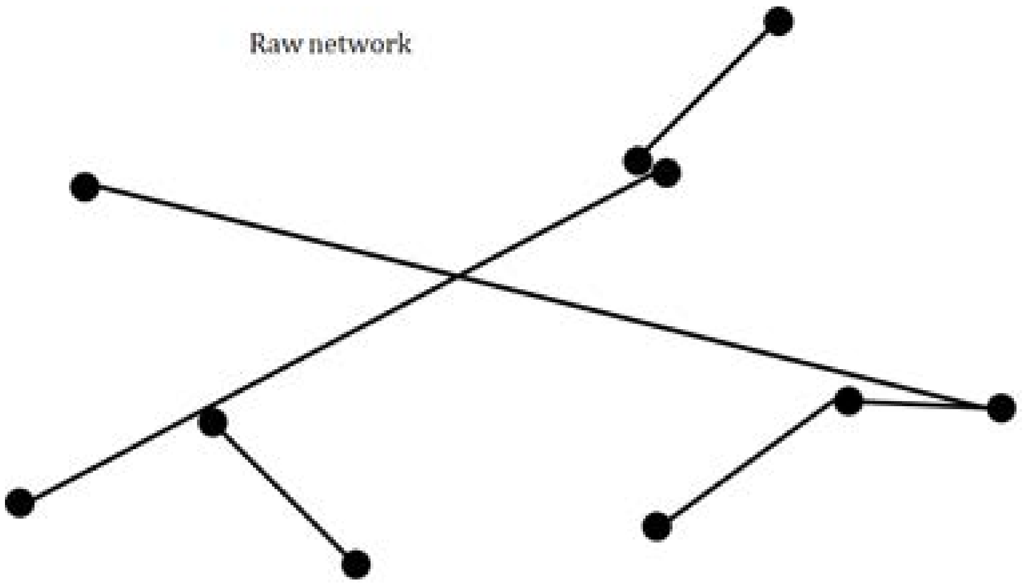
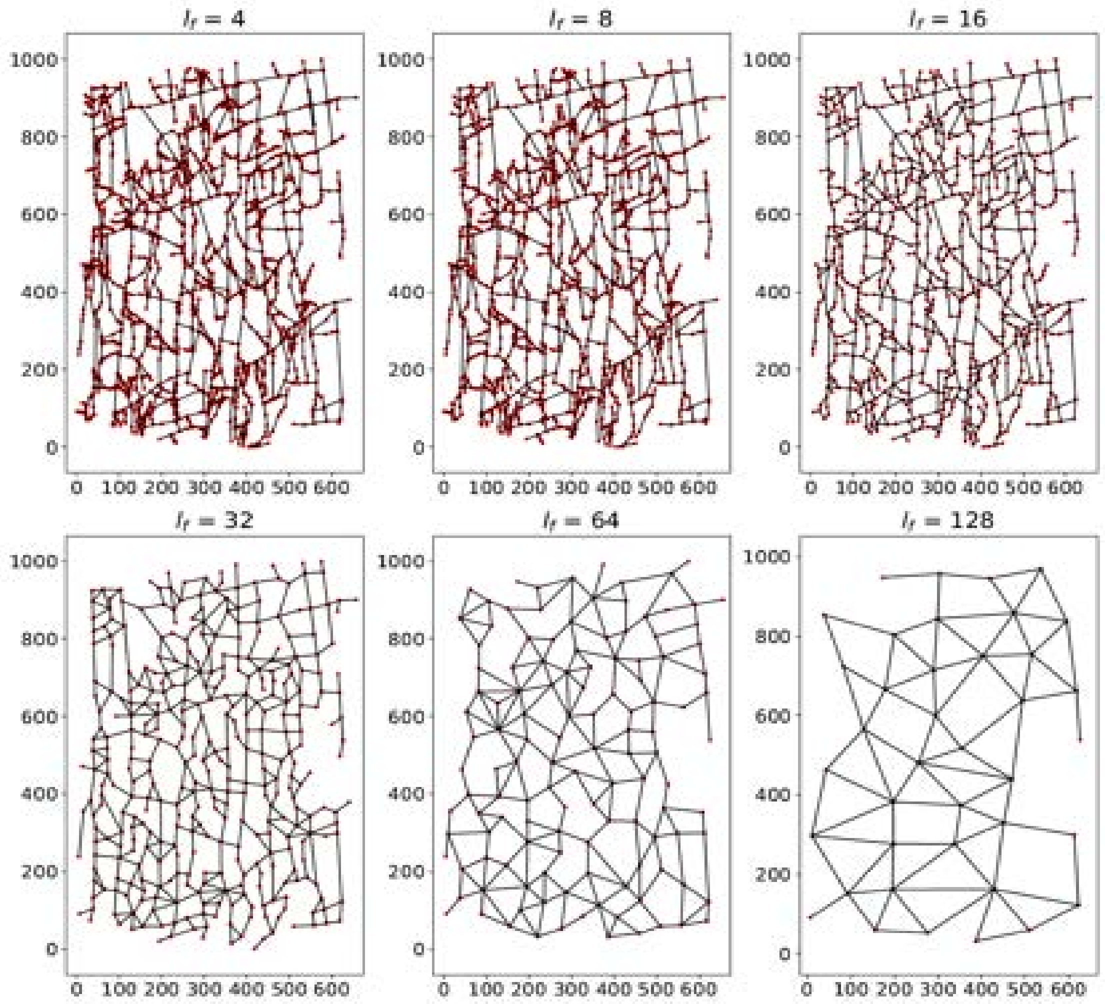
Meshing artifacts





Efficient fracture modeling

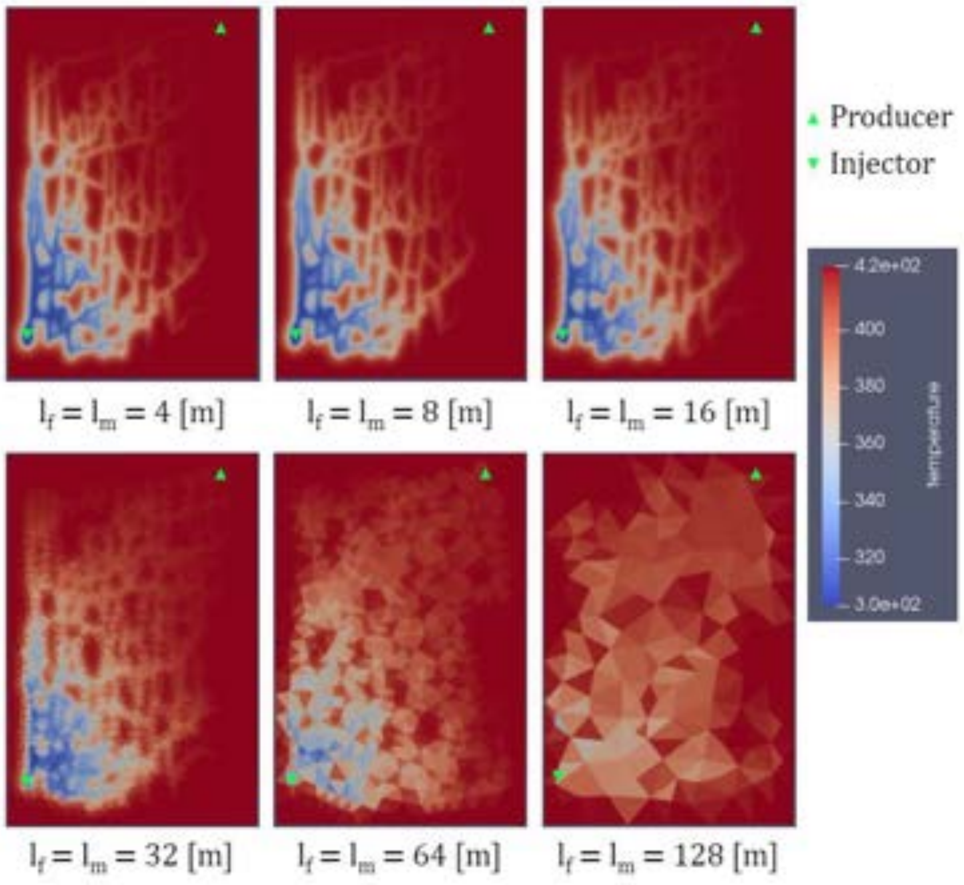




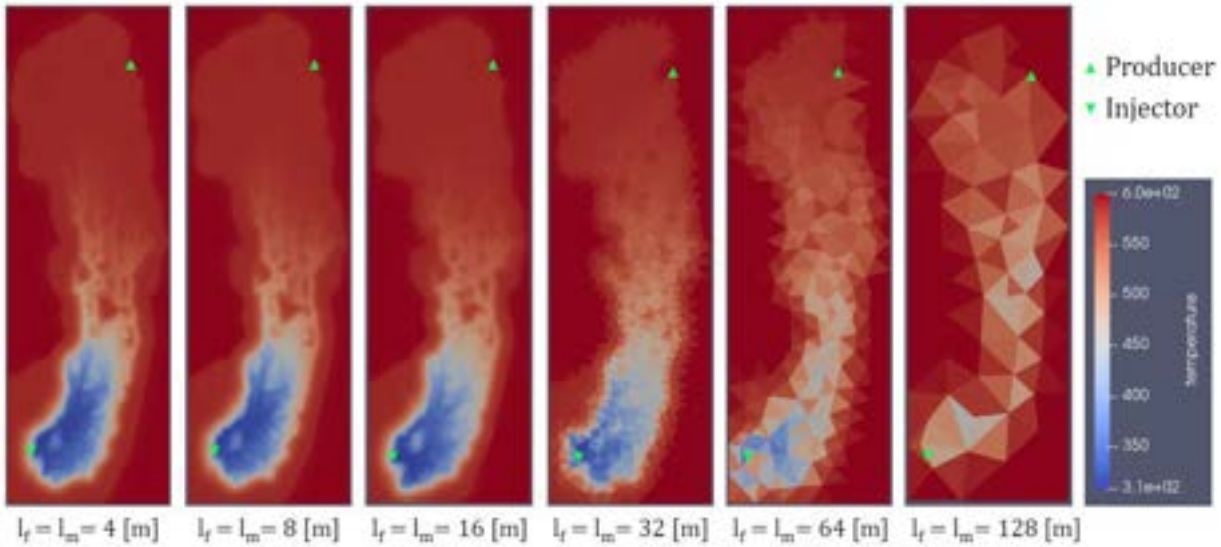
de Hoop et al. (2022)

Sensitivity of geothermal systems

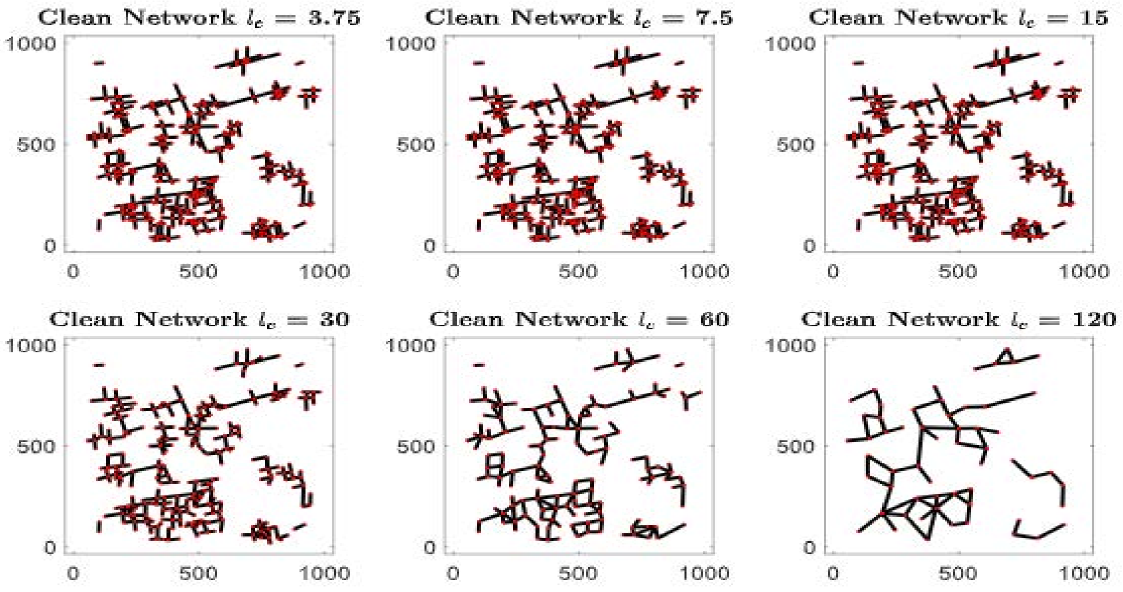
High-enthalpy super critical water

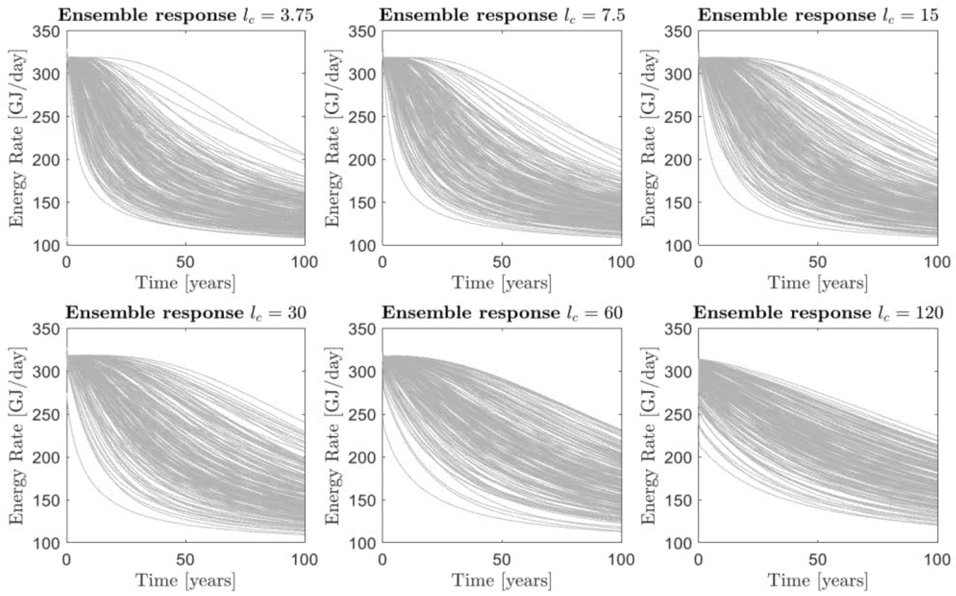


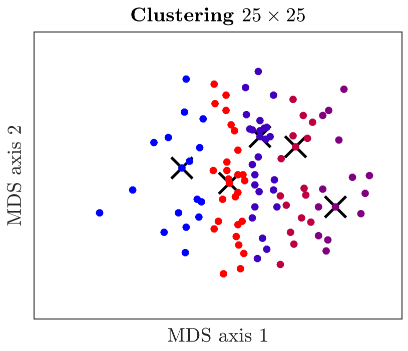
High-enthalpy steam-water system

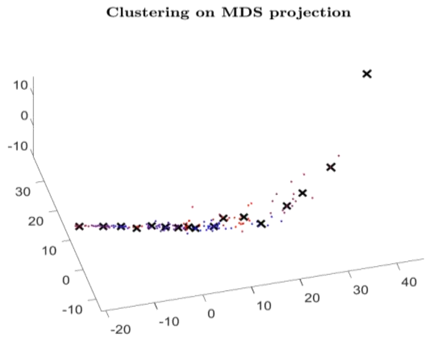


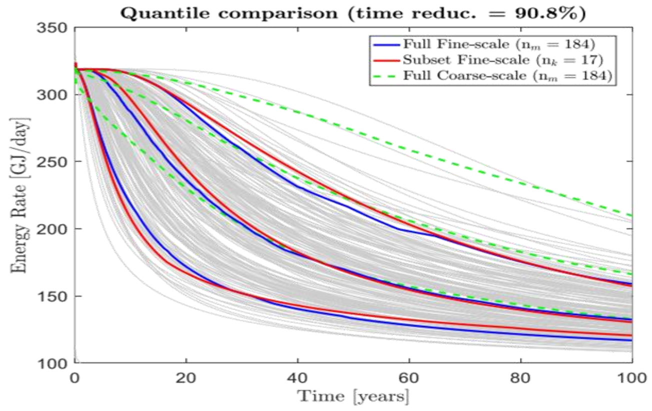
Uncertainty quantification in fractured reservoirs











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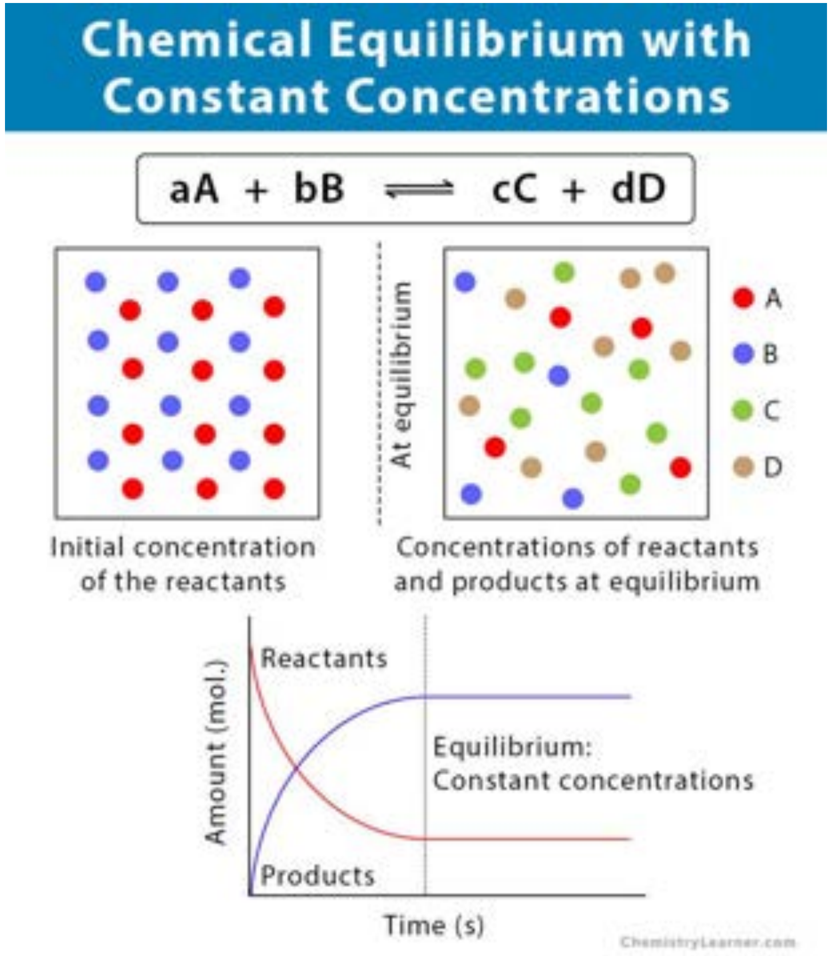
Equilibrium chemical reactions



Component mass balance:

$$\frac{\partial}{\partial t}\left(\phi \sum_{p} \rho_p S_p x_{cp}\right) + \nabla \cdot \sum_{p} \rho_p x_{cp} u_p = \sum_{r=1}^{n_r} v_{c,r} r_r$$

$$\boldsymbol{a_c} + \boldsymbol{l_c} = \boldsymbol{Vr}$$

$$\boldsymbol{a_c} + \boldsymbol{l_c} = \boldsymbol{Vr} \times \boldsymbol{E} \quad \Rightarrow \quad \boldsymbol{a_e} + \boldsymbol{l_e} = \boldsymbol{0}$$

Chemical reactions:

$K_{sp} - Q_{sp} = 0$ equilibrium

$a_c^k + l_c^k = \boldsymbol{vr}^k$ kinetic

Equilibrium reactions in brine-CO_2

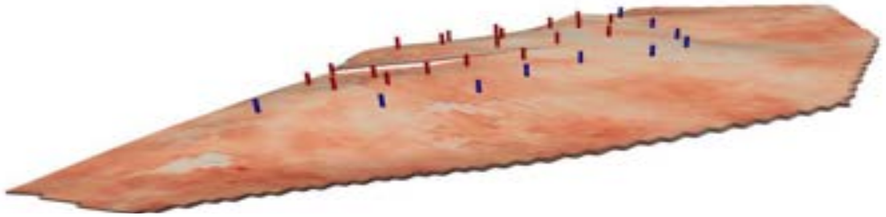
$$\boldsymbol{E} \times \frac{\partial}{\partial t}(\phi \rho_t z_c) + \mathrm{div}(l_c) = \sum_{q=1}^{n_q} v_{cq} r_q$$

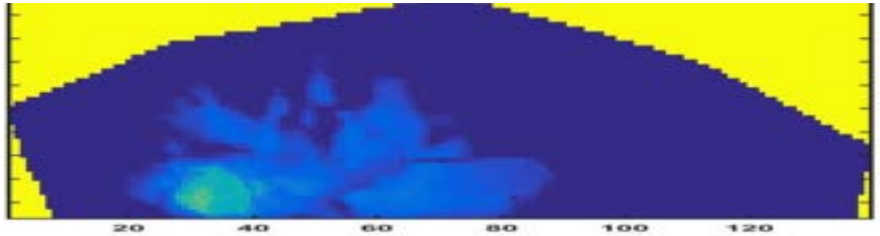
$$f_i^g = f_i^l$$

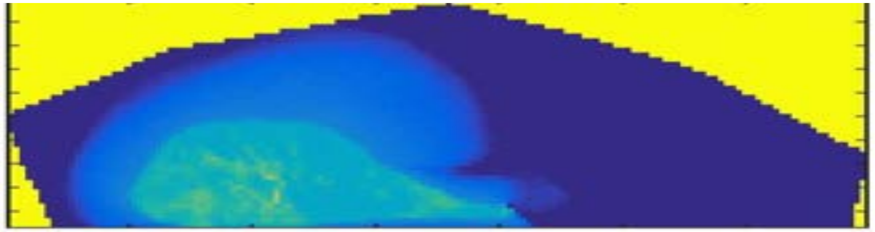
$$\frac{\partial}{\partial t}\left(\phi^T \rho_t^E z_i^E\right) + \mathrm{div}(\boldsymbol{e_i l}) = 0$$

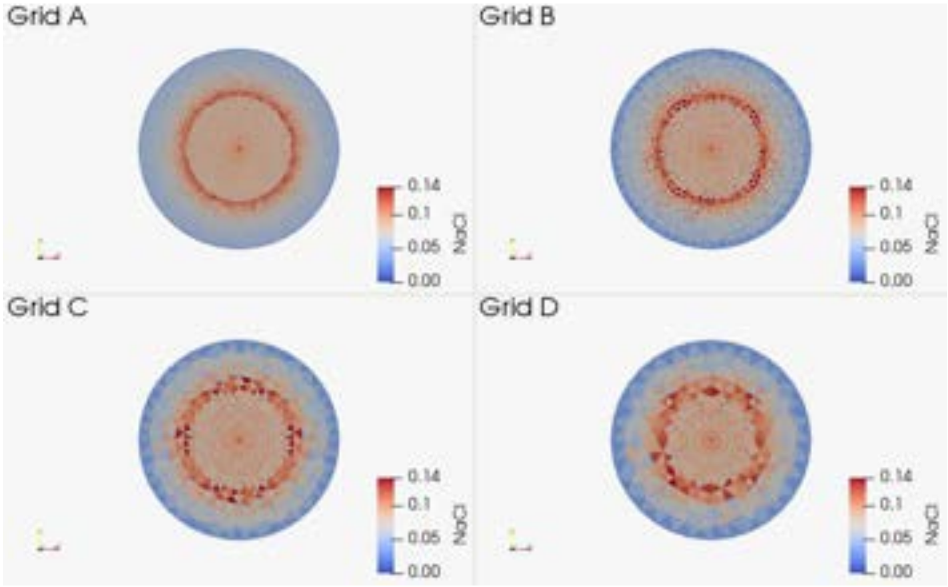
$$f_i^g = f_i^l \qquad \rho_t^E = \rho_t \textstyle\sum_{i=1}^{n_e} \boldsymbol{e_i z}$$

$$\prod_{c=1}^{n_c} a_c^{v_{cq}} - K_q = 0 \qquad \boldsymbol{z^E} \textstyle\sum_{i=1}^{n_e} \boldsymbol{e_i z} - \boldsymbol{Ez} = 0$$









Kala and Voskov, Comput. Geosci, 2020

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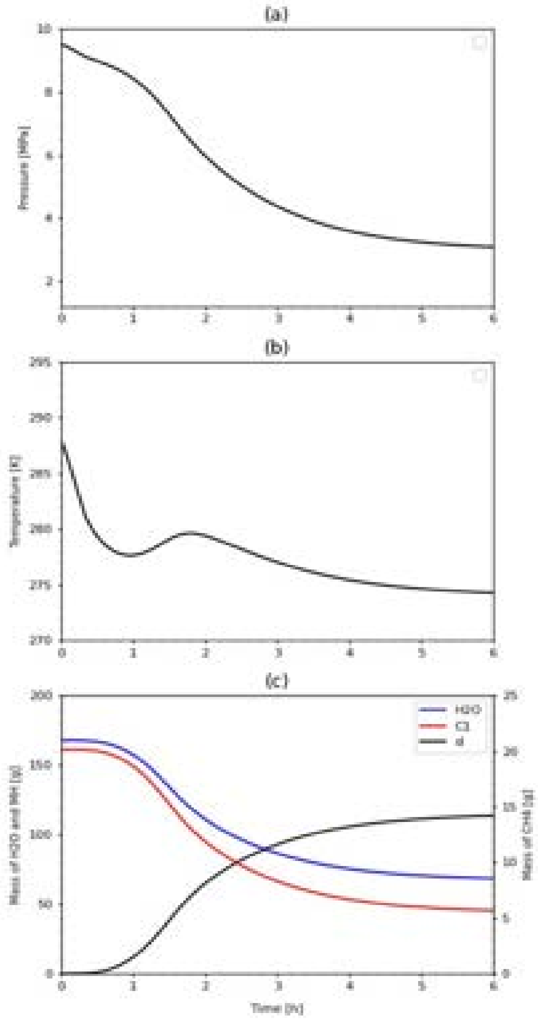
Modeling of hydrate formation

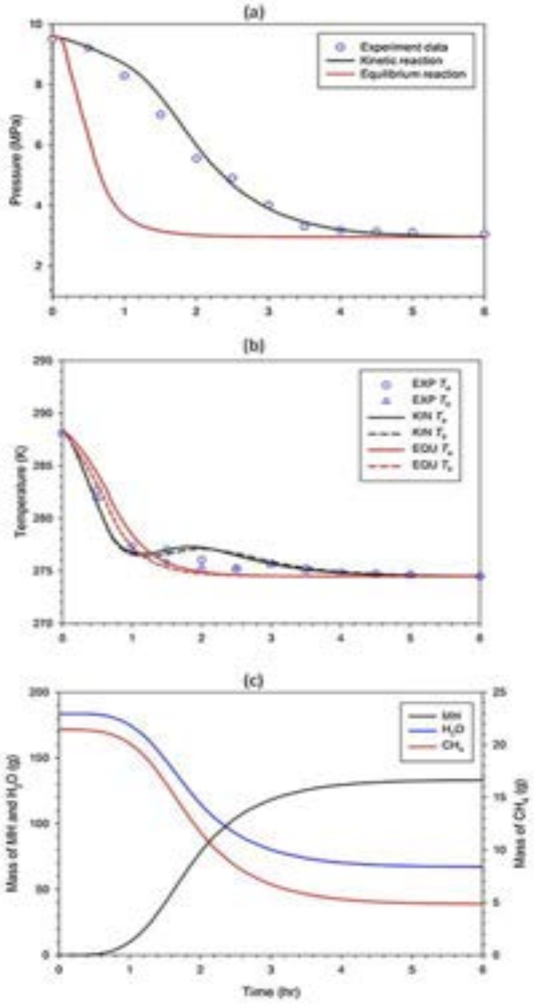
- Numerical simulation of hydrate formation experiment
  - Core filled with brine and free gas CH_4
  - Initially above hydrate formation pressure
  - Cooled down to hydrate formation conditions

- Pressure, temperature and mass recorded over time

DARTS

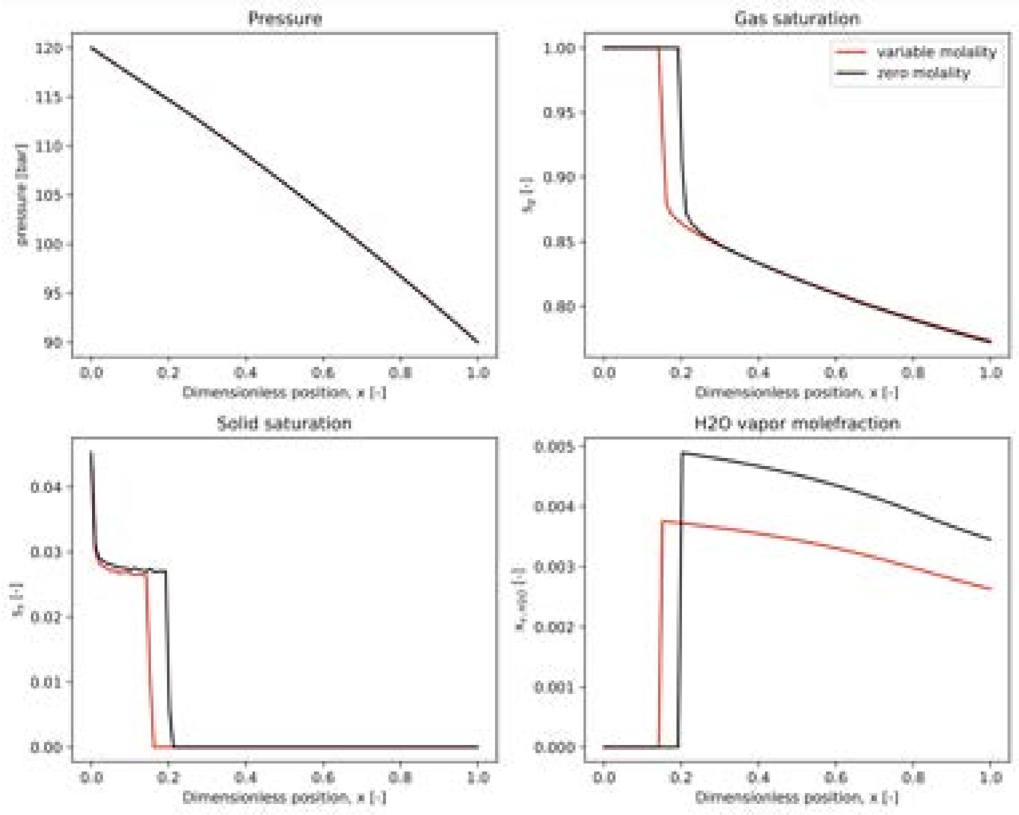


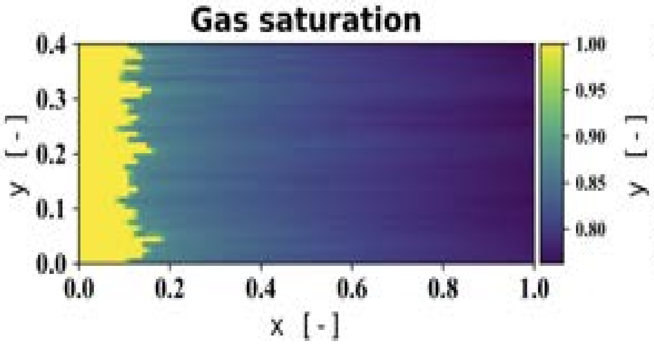
TOUGH+Hydrate

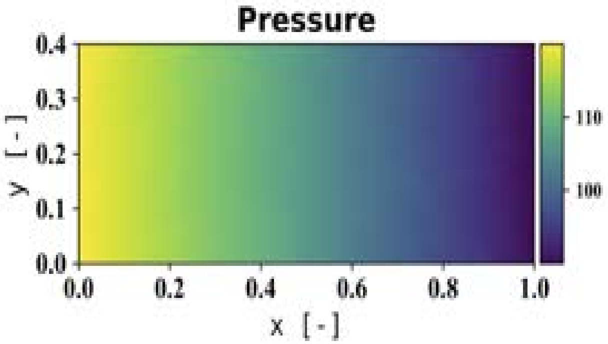


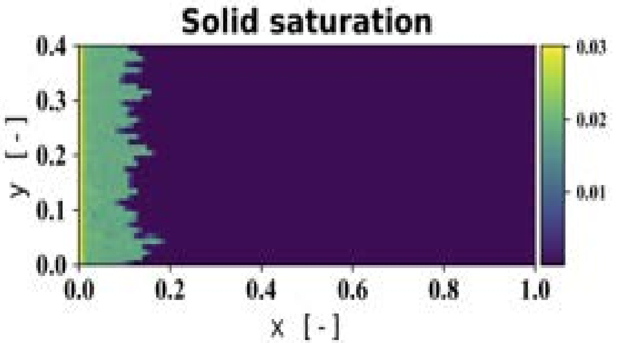
Yin et al., 2013

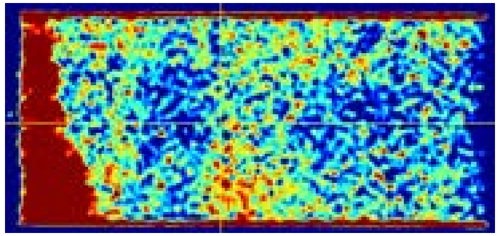
Modeling of salt formation due to dry-out











CO_2 injection into calcite core

- Carbon dioxide dissolution:

$$CO_{2(g)} \rightleftharpoons CO_{2(aq)},$$

- Acid formation:

$$CO_{2(aq)} + H_2O \rightleftharpoons H_2CO_3,$$

$$H_2CO_3 \rightleftharpoons H^+ + HCO_3^-,$$

$$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-},$$

- Calcite dissolution:

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

$$CaCO_3 + H_2CO_3^* \rightarrow Ca^{2+} + 2HCO_3^-,$$

$$CaCO_3 \rightarrow Ca^{2+} + CO_3^{2-}.$$

- Other aqueous reactions considered:

$$H_2O \rightleftharpoons H^+ + OH^-,$$

$$2H_2O \rightleftharpoons O_2 + 4H^+ + 4e^-,$$

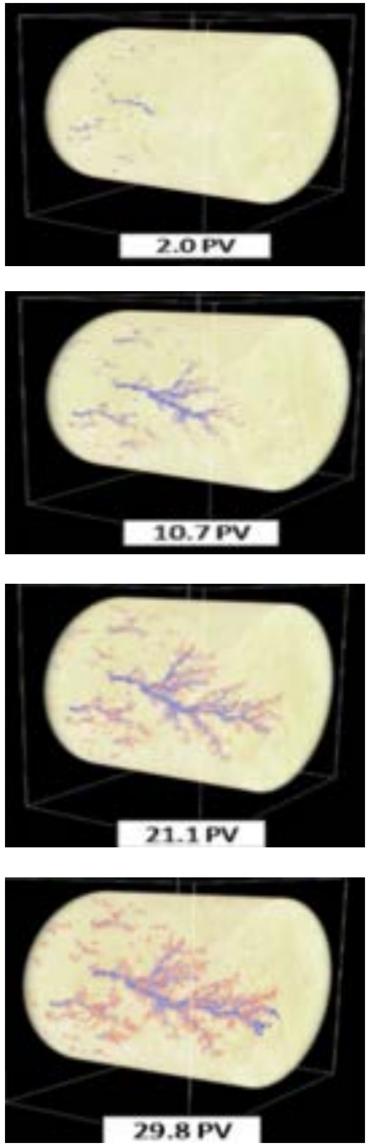
$$2H^+ + 2e^- \rightleftharpoons H_2,$$

$$CO_3^{-2} + 2H^+ \rightleftharpoons CO_2 + H_2O,$$

$$CO_3^{-2} + 10H^+ + 8e^- \rightleftharpoons CH_4 + 3H_2O,$$

$$Ca^{2+} + H_2O \rightleftharpoons CaOH^+ + H^+,$$

$$Ca^{2+} + CO_3^{-2} + H^+ \rightleftharpoons CaHCO_3^+.$$



Snippe et al., IJGGC, 2019

Use PHREEQC for equilibrium chemistry calculation.

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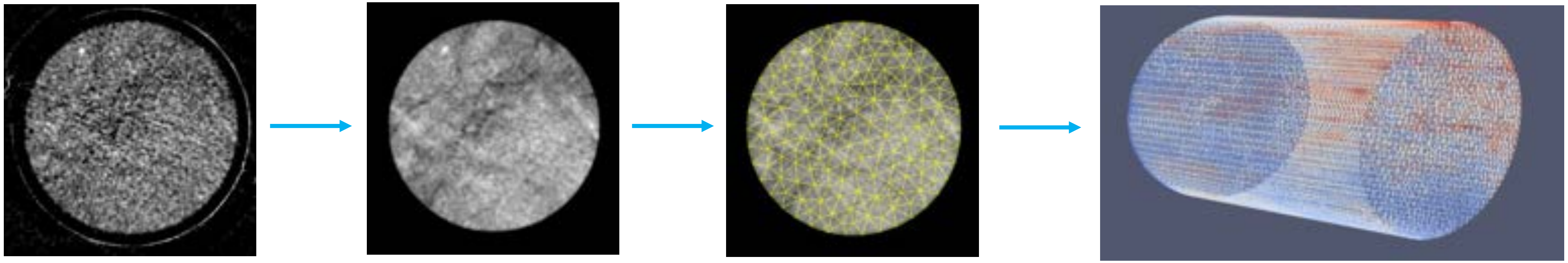
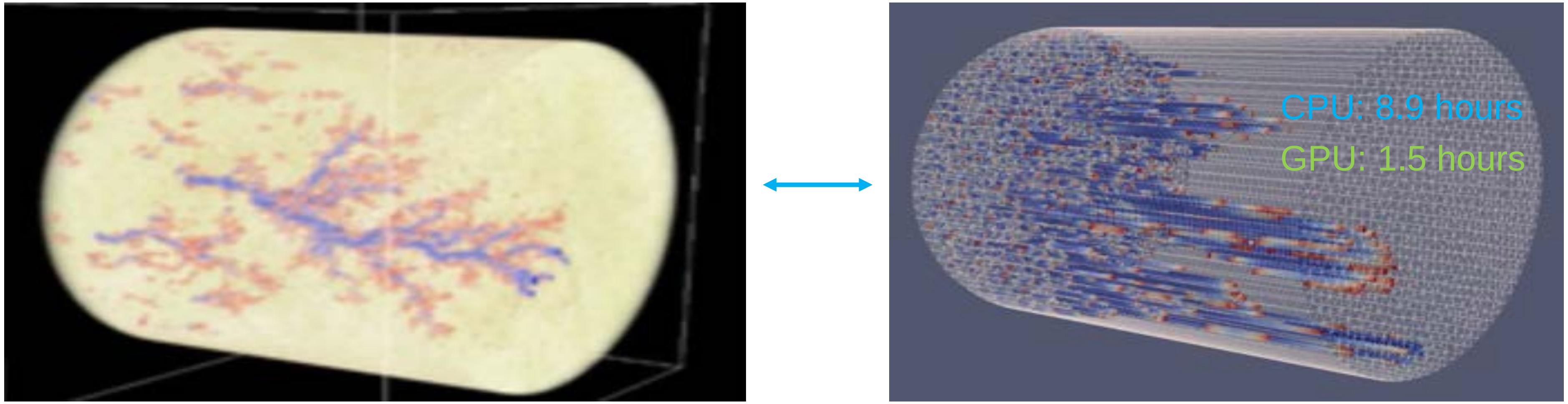
Modeling of dissolution at core scale

Step 1: porosity interpretation (image subtraction, filtering, gridding)



Step 2: modeling of dissolution (combination of DARTS + PHREEQC)



Run time:

8.9 hours (CPU engine)

PHREEQC call: 12 min

Margert, TU Delft, 2019

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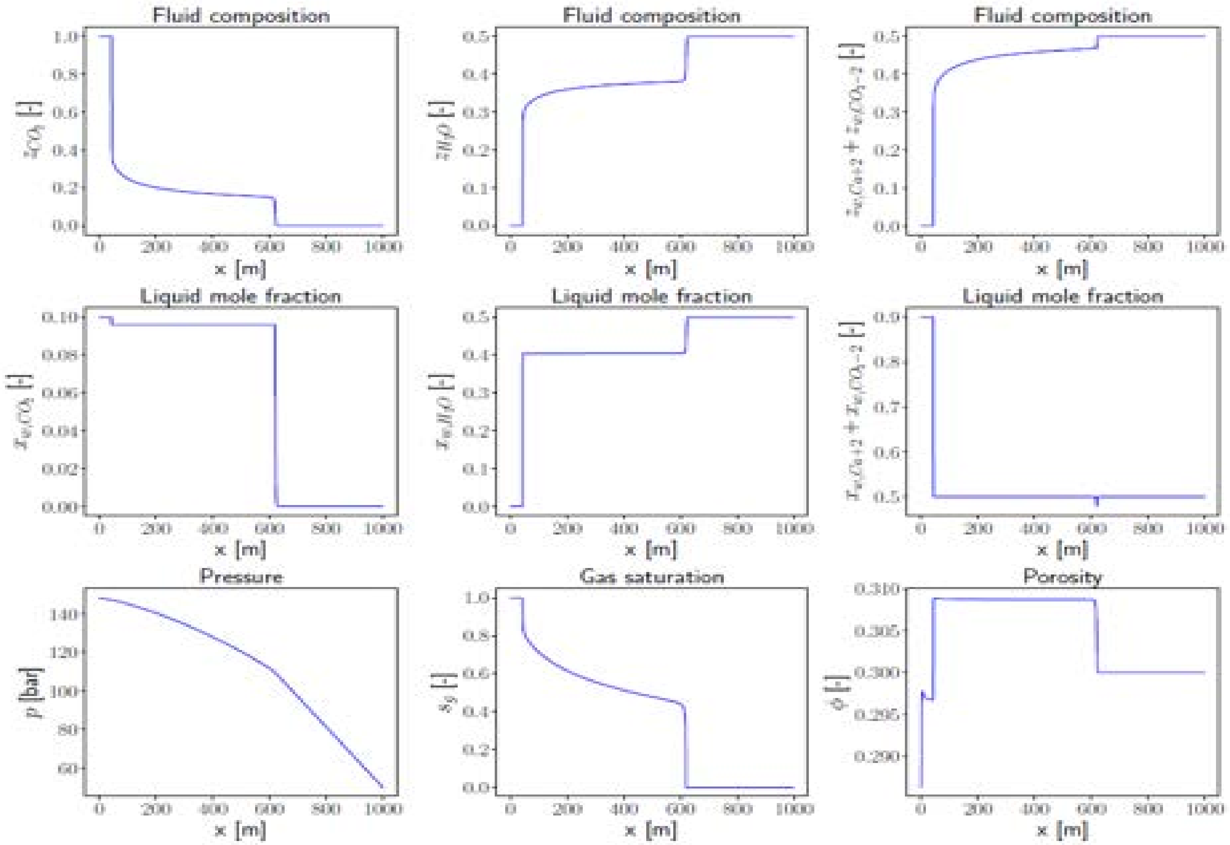
Multiphase flow with reactions (1D benchmark)

$$\frac{\partial n_c}{\partial t} + l_c + q_c = \sum_{k=1}^{K} v_{ck} r_k^K + \sum_{q=1}^{Q} v_{cq} r_q^Q, \quad c = 1, \ldots, C + M,$$

$$n_c = \phi^T \sum_{j=1}^{P} (\rho_j s_j x_{cj}), \quad c = 1, \ldots, C.$$

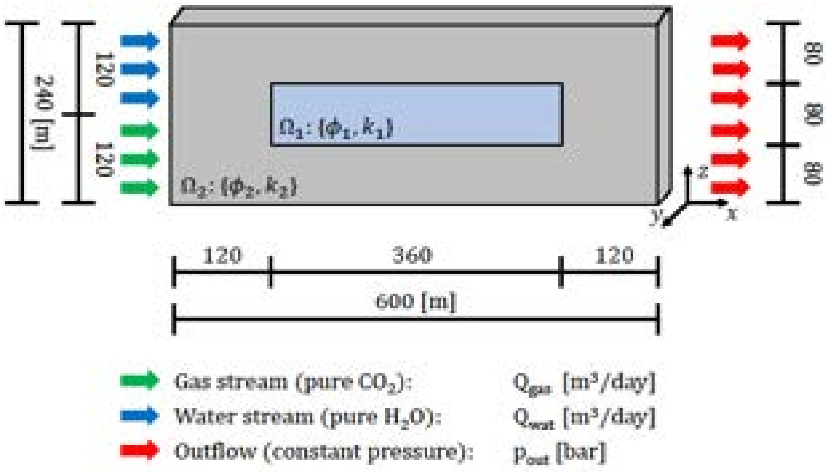
$$n_m = \phi^T \rho_m z_m, \quad m = C + 1, \ldots, M.$$

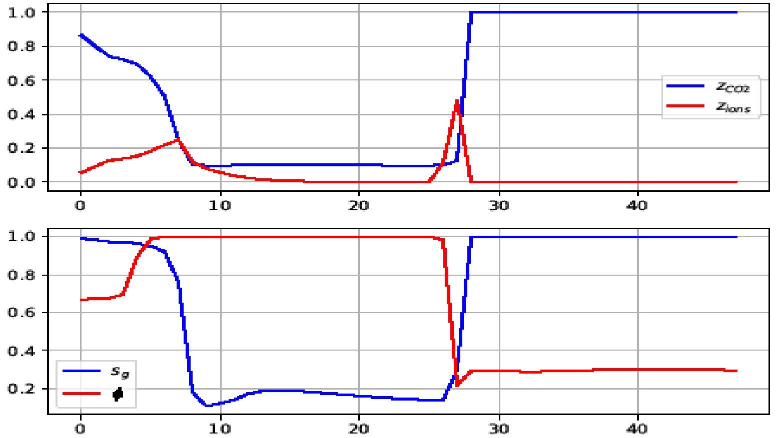
$$\phi = \phi^T \left(1 - \sum_{m=1}^{M} \hat{s}_m\right) \quad k = k_0 \left(\frac{\phi}{\phi_0}\right)^A$$

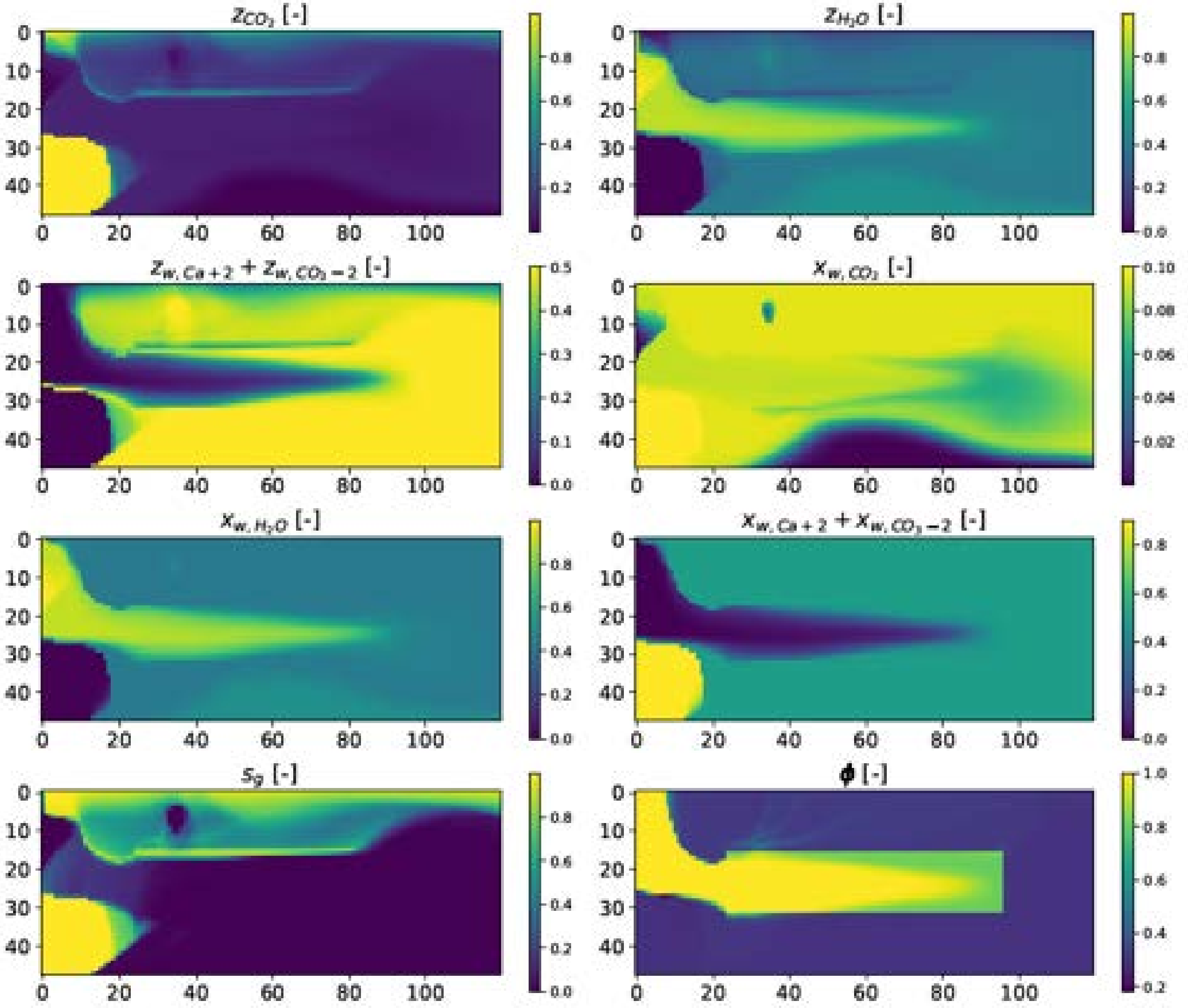


de Hoop et al., SITRAM, 2023

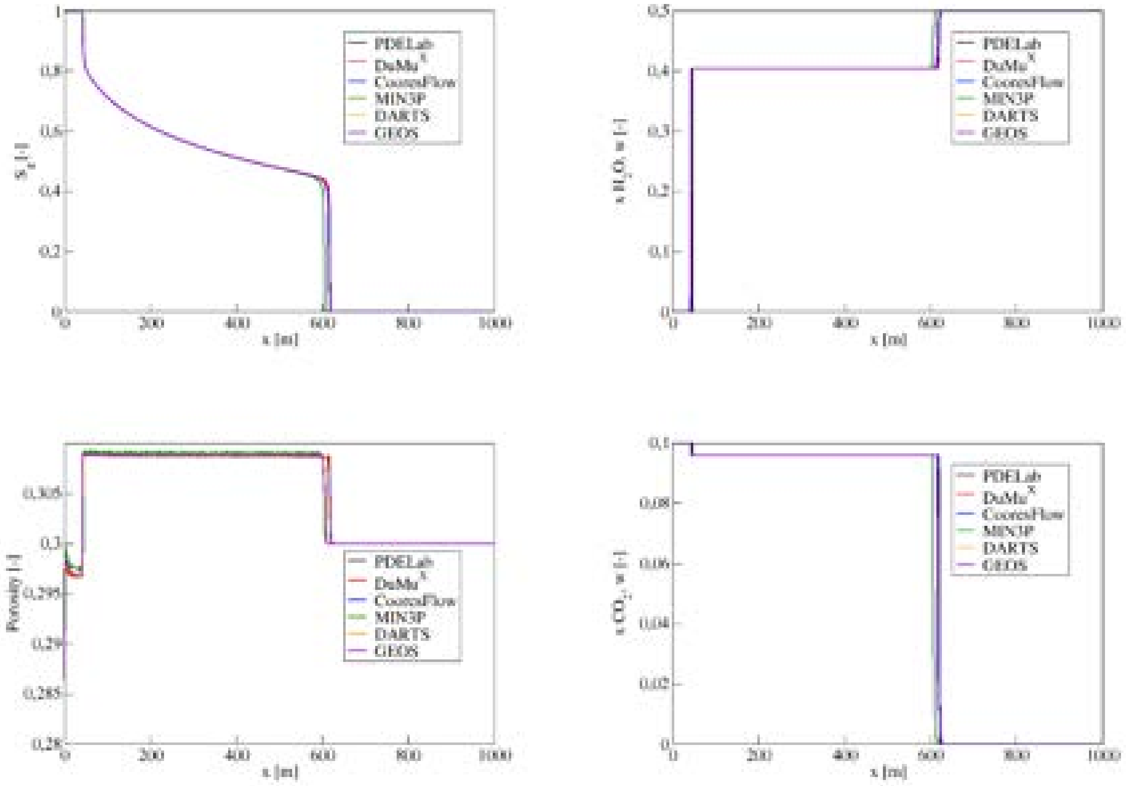
Two-dimensional benchmark

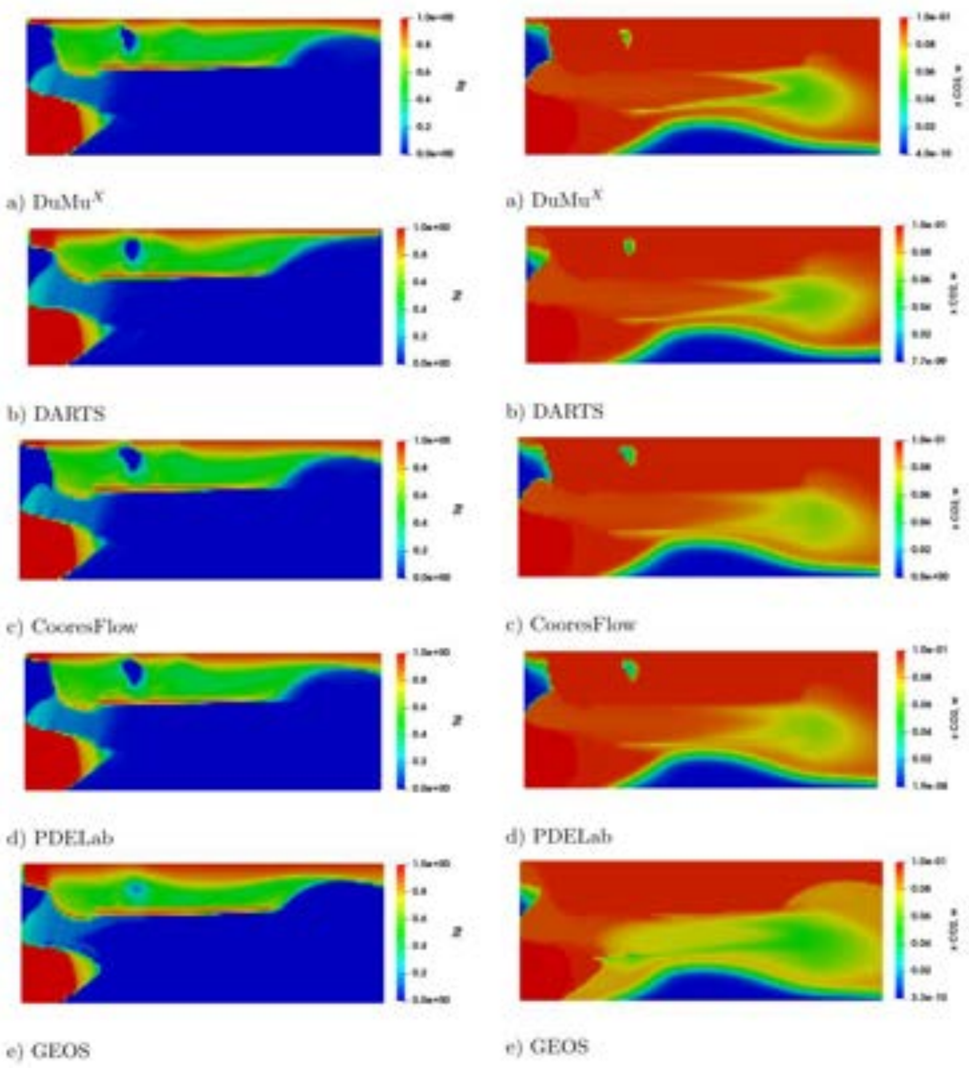






Comparison of different simulators





Ahusborde et al., SITRAM, 2023

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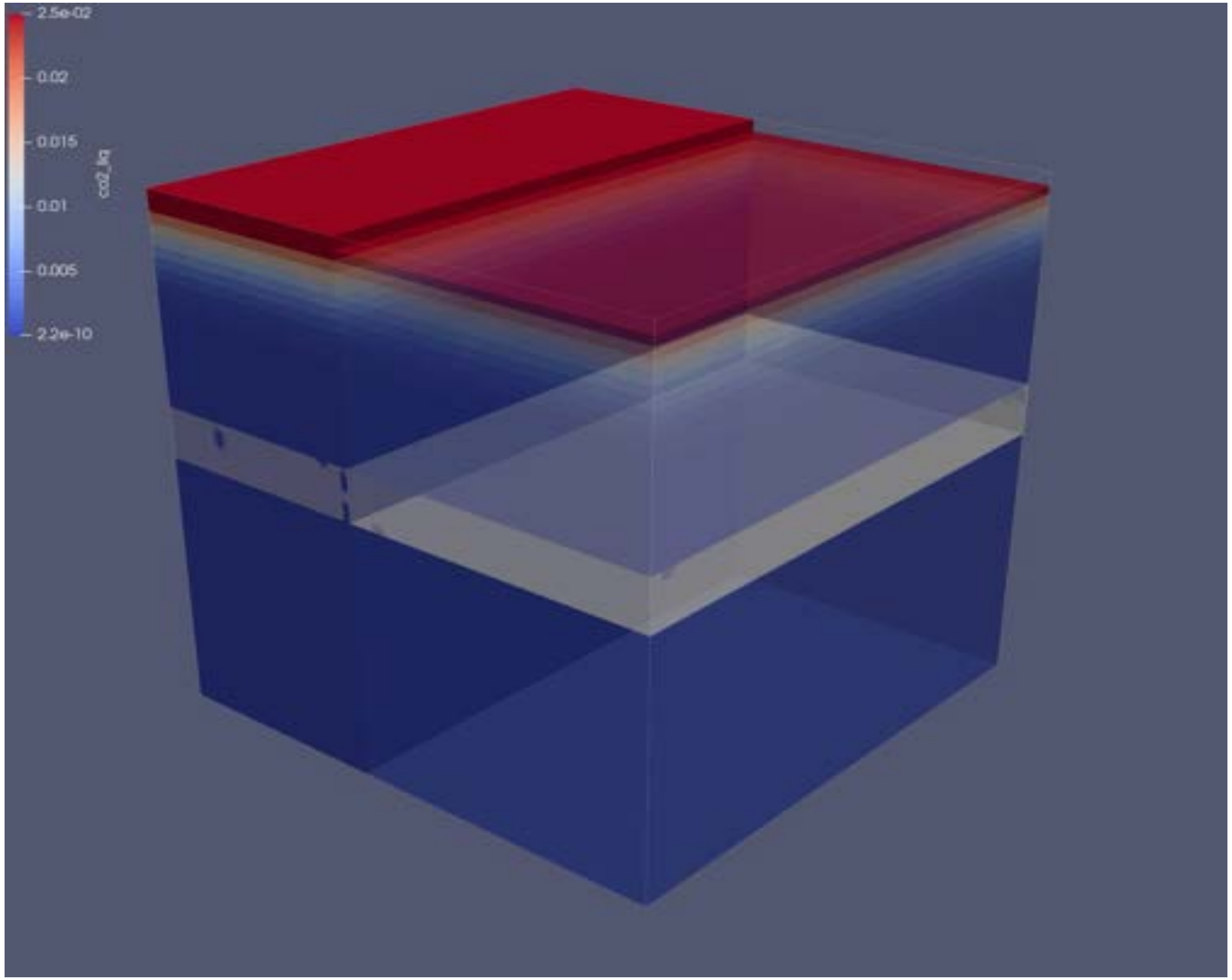
Combined dissolution



Acknowledgments

- DARTS team: Xiaocong Lyu, Mark Khait, Michiel Wapperom, Yang Wang, Aleks Novikov, Stephan de Hoop, Xiaoming Tian, Kiarash Mansour Pour

NWO

TotalEnergies

[For more details on DARTS, check: https://darts.citg.tudelft.nl/](https://darts.citg.tudelft.nl/)

Time for Questions and Answers