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UNIVERSITÉ DE LORRAINE

1st DuMu^X User Meeting

Hydrodynamic and Bio-chemical Effects during Underground Hydrogen Storage

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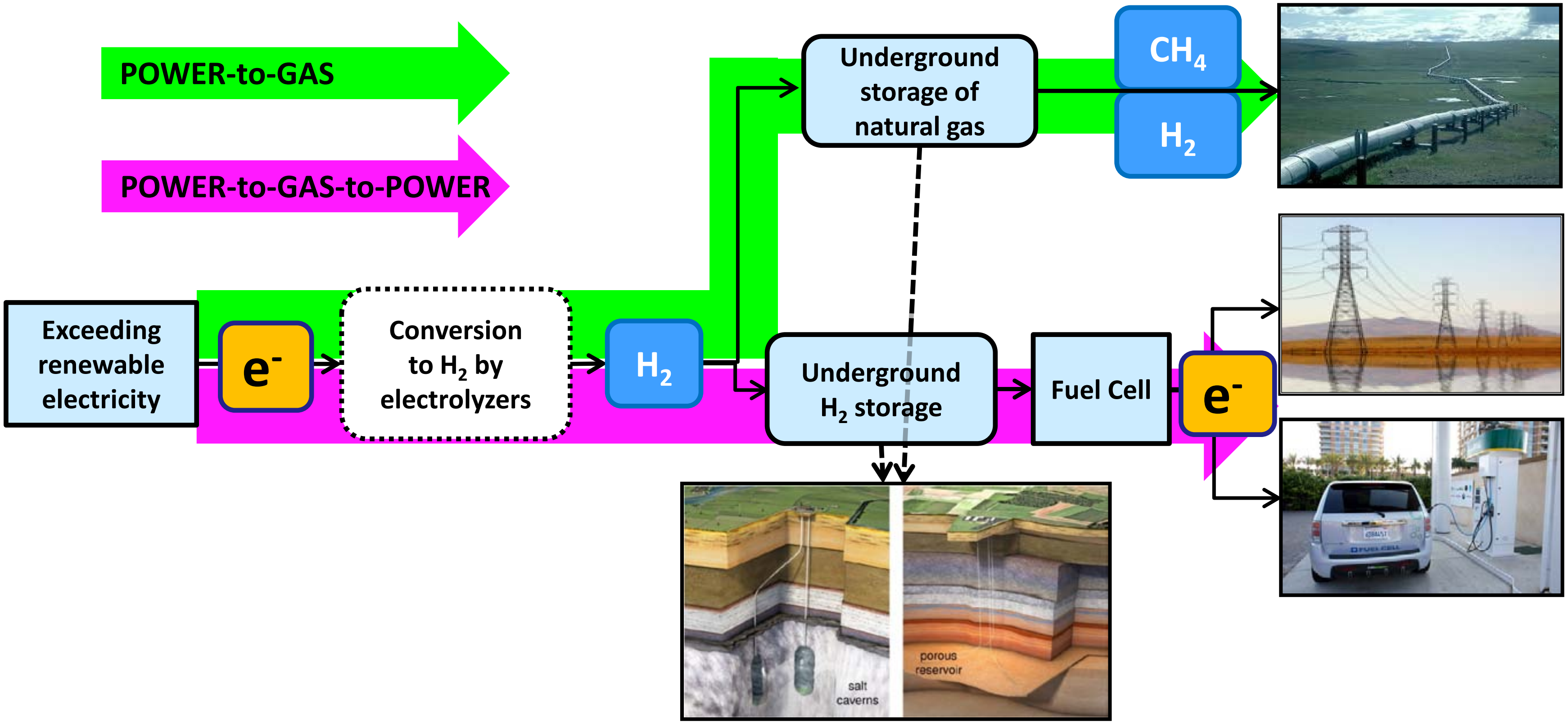
OUTLINE

- INTRODUCTION
- MAIN PHENOMENA IN UHS:
  - Hydrodynamic effects
  - Bio-chemical effects
- MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT
- NUMERICAL IMPLEMENTATION
- CASE STUDIES
- CONCLUSIONS

INTRODUCTION

- Fluctuating supply of renewable energy from wind mills and solar
- Demanding high storage capacities for electrical energy



H2STORE PROJECT

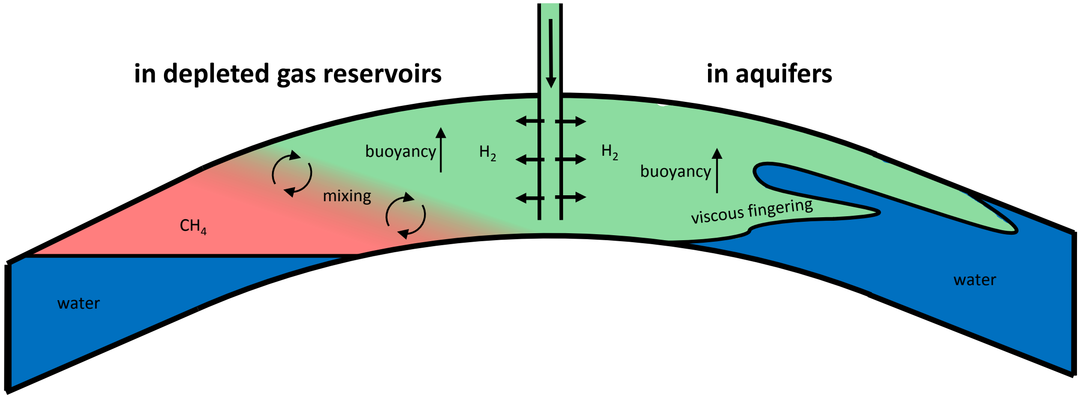
- Started in the mid of 2012 for 3 years duration
- Initiator/financing: German Federal Ministry for Education and Research (BMBF)
- Partnerships:
  - University of Jena
  - Clausthal University of Technology
  - GFZ Potsdam
  - University of Lorraine/CNRS
- Aims to investigate the feasibility of large-scale hydrogen storage in porous geological formations
- Subproject: Numerical simulation of gas mixing processes during underground hydrogen storage
- Goal: Numerical model for coupled hydrodynamic and bio-chemical effects in UHS

MAIN PHENOMENA IN UNDERGROUND HYDROGEN STORAGE

HYDRODYNAMIC EFFECTS

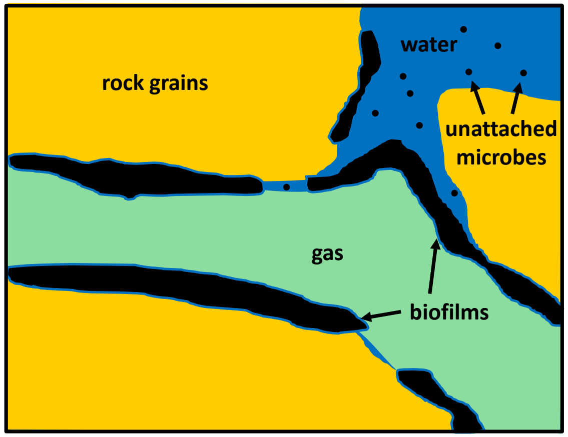
- In depleted gas reservoirs
  - Mixing of initial and injected gases
  - Gravity segregation
  - Lateral spreading

- In aquifers
  - Viscous fingering
  - Gravity overriding
  - Lateral spreading



BIO-CHEMICAL EFFECTS

- H_2 is an electron donor for the metabolism of several anaerobic microbial species
  - Methanogenetic archaea
  - Acetogenic archaea
  - Sulfate-reducing bacteria
  - Iron-reducing bacteria



- Large changes in the gas composition were observed in town gas (~50% H_2) storages
  - Underground methanation by Sabatier's reaction:

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

- **Population dynamics** for 2 microbial species: (M) Methanogenic archaea, (S) Sulfate-reducing bacteria

$$\frac{\partial n_m}{\partial t} = \psi_m^{growth} S_w n_m - \psi_m^{decay} n_m + \nabla \cdot \left(D_m \nabla n_m \right)$$

- **Reactive transport** for 6 mobile components: H_2, CO_2, CH_4, H_2O, SO_4^{2-}, H_2S

$$\phi \frac{\partial \left(\rho_g C_g^k S_g + \rho_w C_w^k S_w \right)}{\partial t} - \nabla \cdot \left(\rho_g C_g^k \frac{K k_{rg}}{\mu_g} \cdot \left(\nabla P_g - \rho_g g \right) + \rho_w C_w^k \frac{K k_{rw}}{\mu_w} \cdot \left(\nabla P_w - \rho_w g \right) \right)$$
$$- \nabla \cdot \left(\phi D_g^k \rho_g S_g \nabla C_g^k + \phi D_w^k \rho_w S_w \nabla C_w^k \right) = \phi S_w \sum_m \gamma_m \frac{\psi_m^{growth}}{Y_m} n_m$$

Bio-reaction term

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MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

- Bio-chemical reactions
  - Methanogenesis: $$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$
  - Sulfate-reduction: $$SO_4^{2-} + 5H_2 \rightarrow H_2S + 4H_2O$$
- Stoichiometric coefficients

$$\gamma_M = \begin{pmatrix} -4 \\ -1 \\ 1 \\ 2 \\ 0 \\ 0 \end{pmatrix} \qquad \gamma_S = \begin{pmatrix} -5 \\ 0 \\ 0 \\ 4 \\ -1 \\ 1 \end{pmatrix}$$

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MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

- Microbial growth functions (Monod model)
  - for methanogenic archaea

$$\psi_M = \psi_{\max} \left(\frac{C_w^{H_2}}{\alpha_{1,M} + C_w^{H_2}} \right) \left(\frac{C_w^{CO_2}}{\alpha_{2,M} + C_w^{CO_2}} \right)$$

  - for sulfate-reducing bacteria

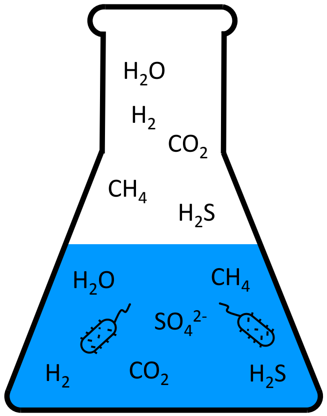
$$\psi_S = \psi_{\max} \left(\frac{C_w^{H_2}}{\alpha_{1,S} + C_w^{H_2}} \right) \left(\frac{C_w^{SO_4^{2-}}}{\alpha_{2,S} + C_w^{SO_4^{2-}}} \right)$$

- Other growth models were tested

NUMERICAL IMPLEMENTATION

DuMu^X IMPLEMENTATION (*2p6c2mo*)

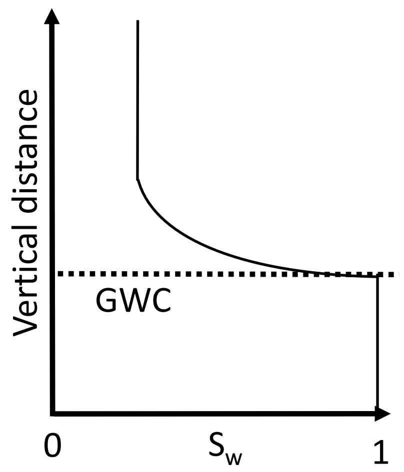
- Based on implicit 2p2c model
- New fluidsystem
  - 2 phases
  - 6 components: H_2O, H_2, CO_2, CH_4, SO_4^{2-}, H_2S (SO_4^{2-} not in thermodynamic equilibrium)
  - 2 microbial species: Methanogenic archaea and sulfate-reducing bacteria
  - Introduction of new components (H_2S, SO_4^{2-}), binary coefficients, a microbe index and a method for microbial diffusion coefficient



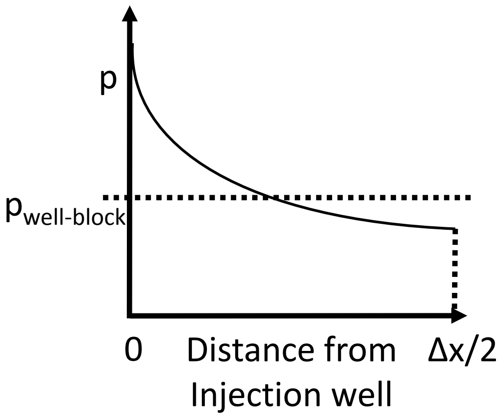
- Extension of the model (*2p6c2mo*)
  - Gradients and effective diffusion coefficients for additional components and microbes added (*2p6c2mofluxvariables.hh*)
  - Volume variables extended for additional components and microbes (*2p6c2movolumevariables.hh*)
  - Equations for additional components and microbial population dynamics added, bio-reaction term added in *computeSource(…)* (*2p6c2molocalresidual.hh*)

PROBLEM DEFINITION

- Reservoir initialization (*initialAtPos(…)*)
  - Hydrostatic equilibrium
  - Gas zone (pressure gradient depends on gas density)
  - Gas/water zone (each phase has its own pressure gradient, S_w calculated on p_c)
  - Water zone (pressure gradient depends on water density)

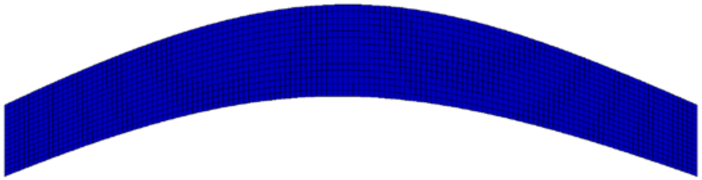


- Injection/production of fluids by wells (*solDependentSource(…)*)
  - Either rate controlled (injected phase is known, produced phase depends on mobility in the well-block)
  - Or bottom-hole pressure controlled by using Peaceman's well model (injection/production rate is a function of the difference between the defined BHP and the actual well-block pressure)

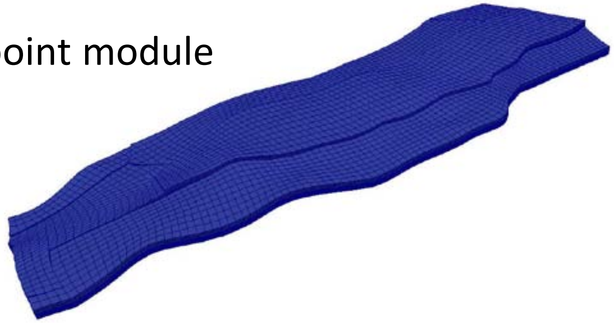


GRID GENERATION

- 2D conceptual reservoir models
  - COMSOL Multiphysics mesh generator (conforming quadrangle grid)
  - Matlab code for conversation into ALUGrid format
  - Imported with dune-alugrid module



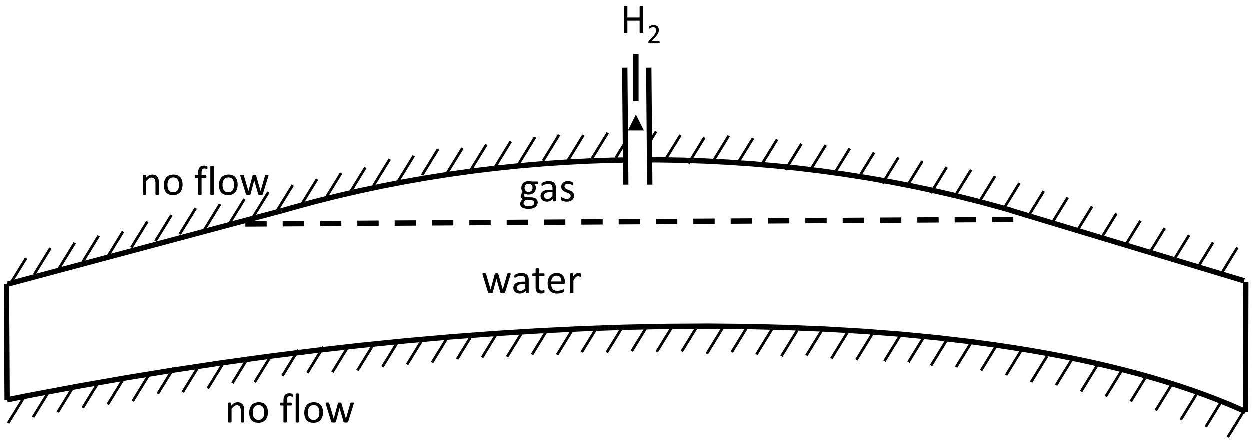
- 3D realistic reservoir models
  - Created in Petrel (non-conforming corner-point grid)
  - Exported as ECLIPSE data file
  - Imported with OPM parser and dune-cornerpoint module



CASE STUDIES

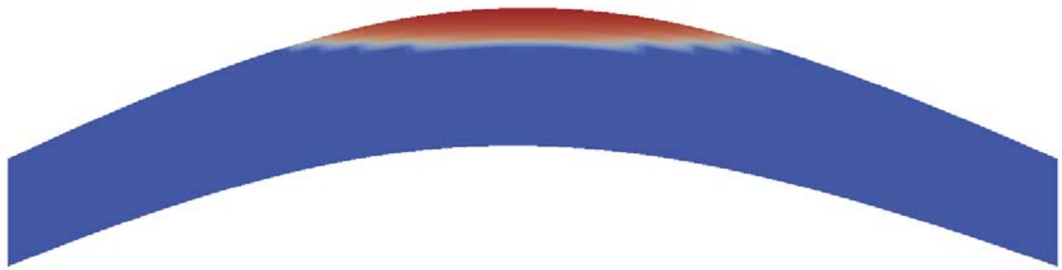
INITIAL AND BOUNDARY CONDITIONS

- 2D Geometry: Dome-shaped anticline formation
- Initially: Hydrostatic equilibrium
- Initial gas composition: 100% H_2
- Hydrogen injection into the top center
- Investigation of different injection rates

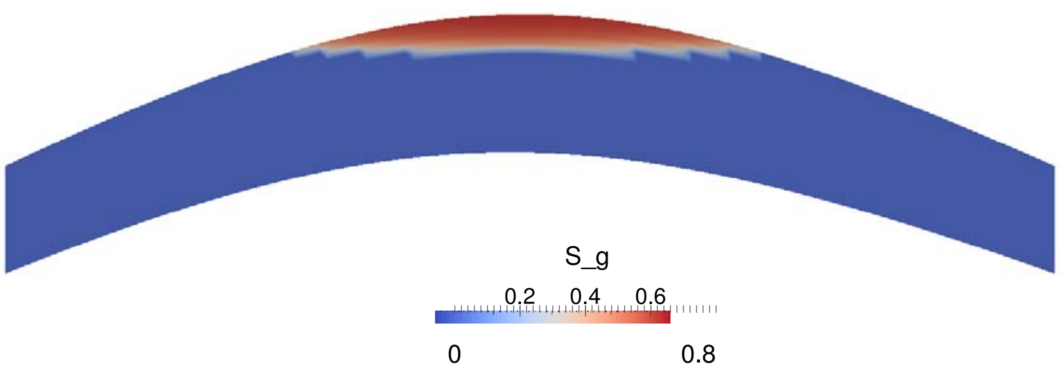


HYDRODYNAMIC EFFECTS

- Hydrogen injection into an reservoir containing an initial amount of hydrogen
  - Stable displacement when hydrogen is injected slow



  - Instable displacement when hydrogen is injected fast



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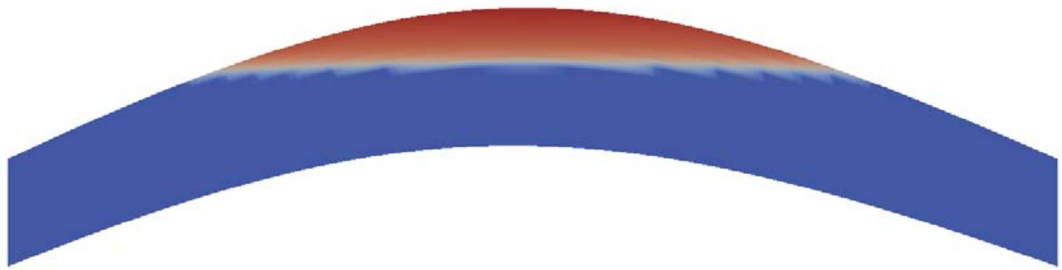

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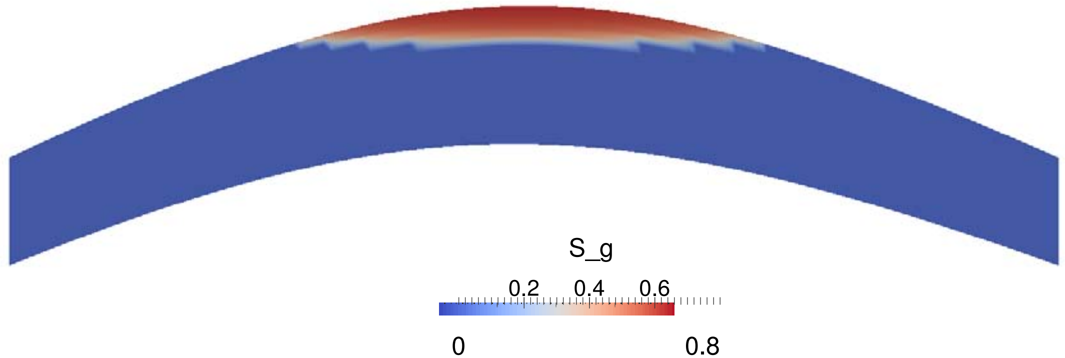

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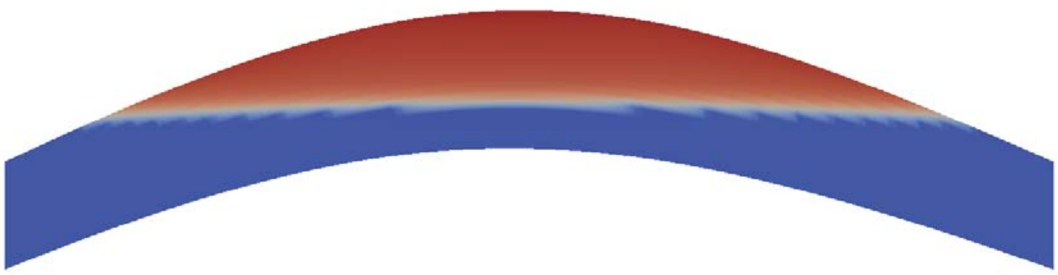

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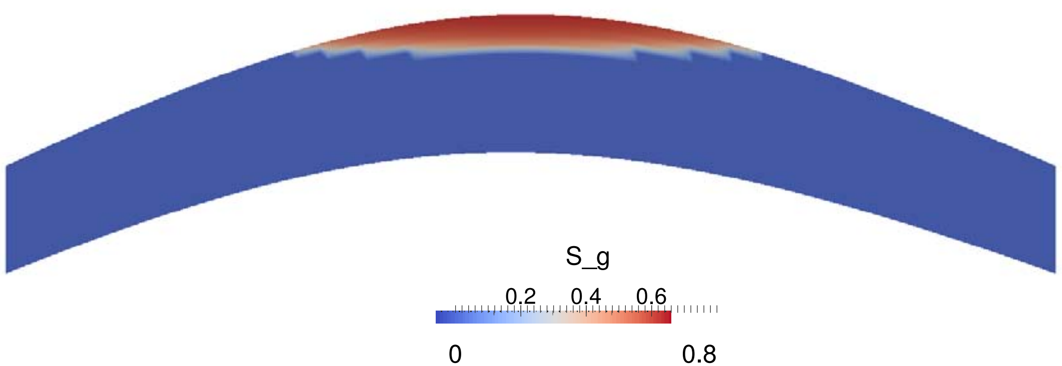

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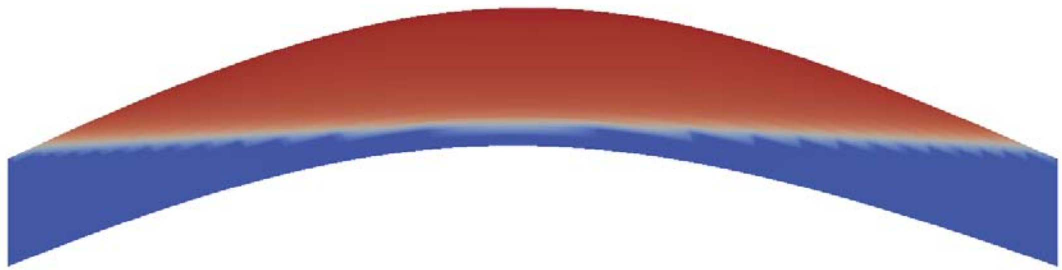

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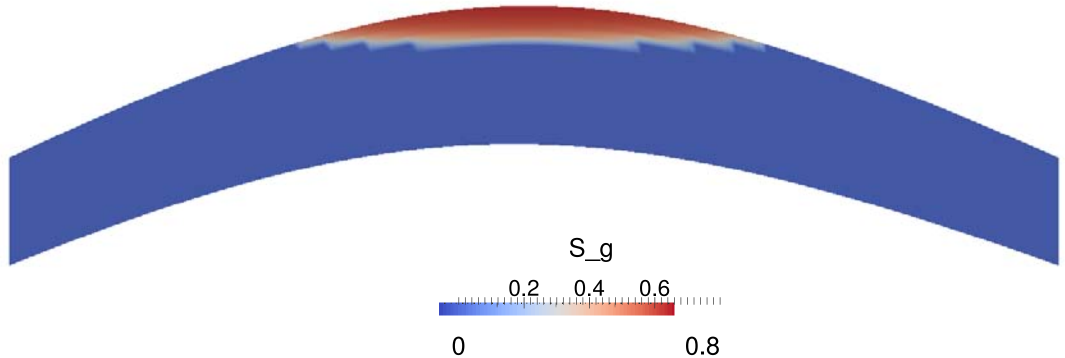

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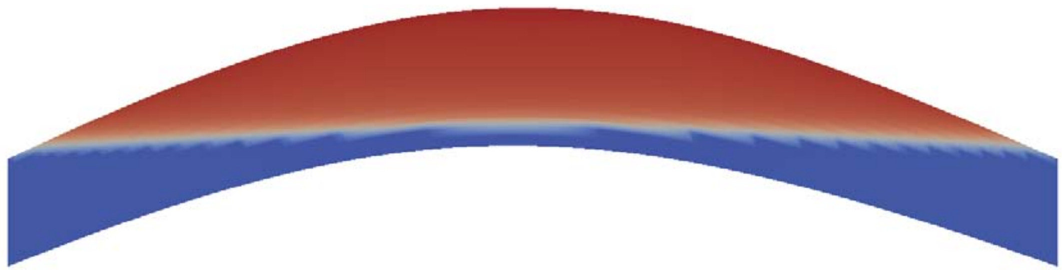

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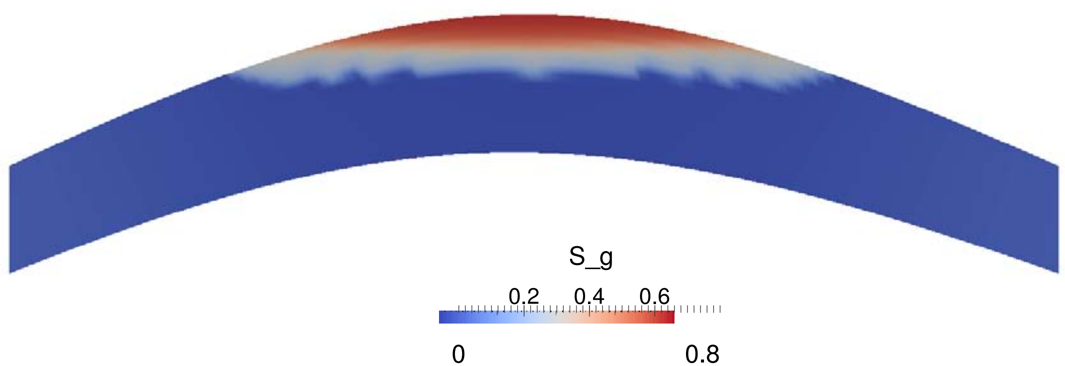

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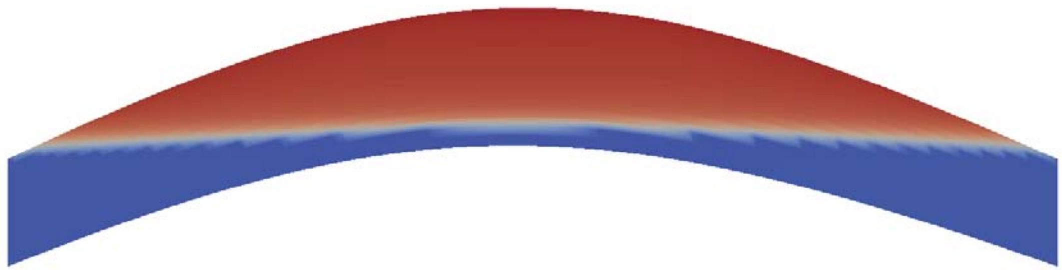

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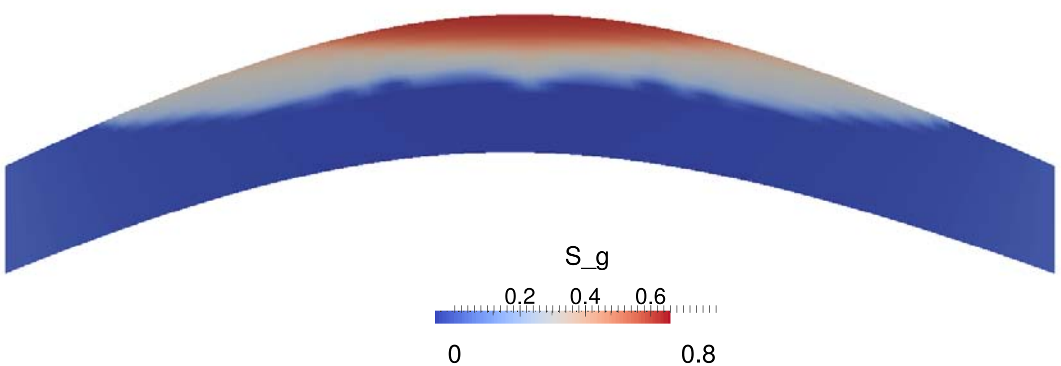

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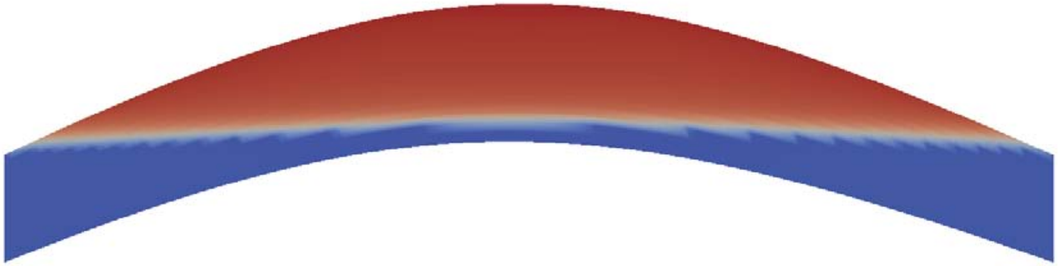

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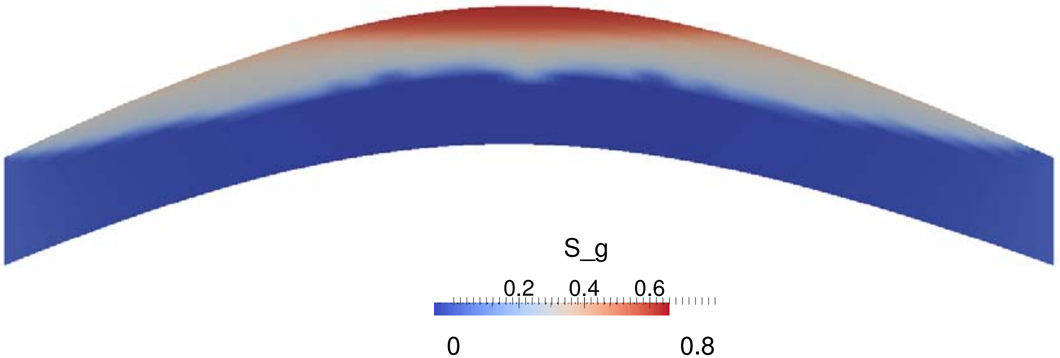
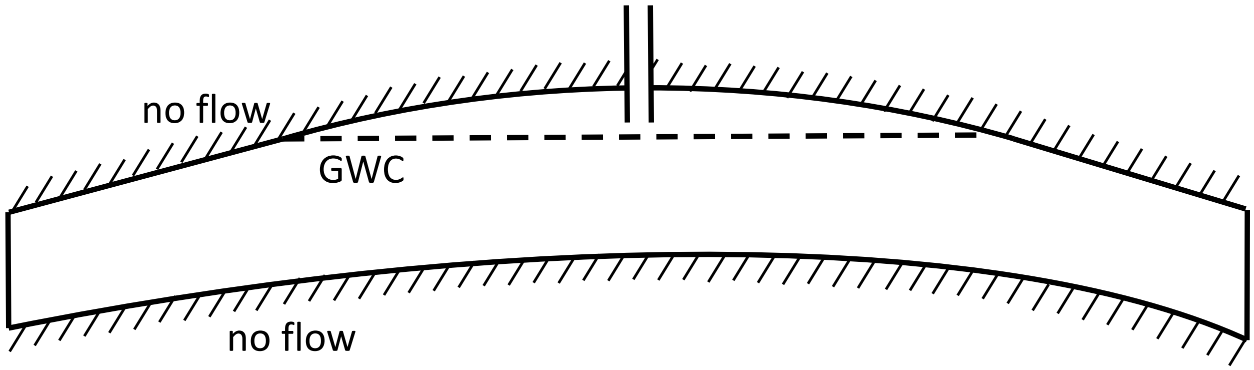


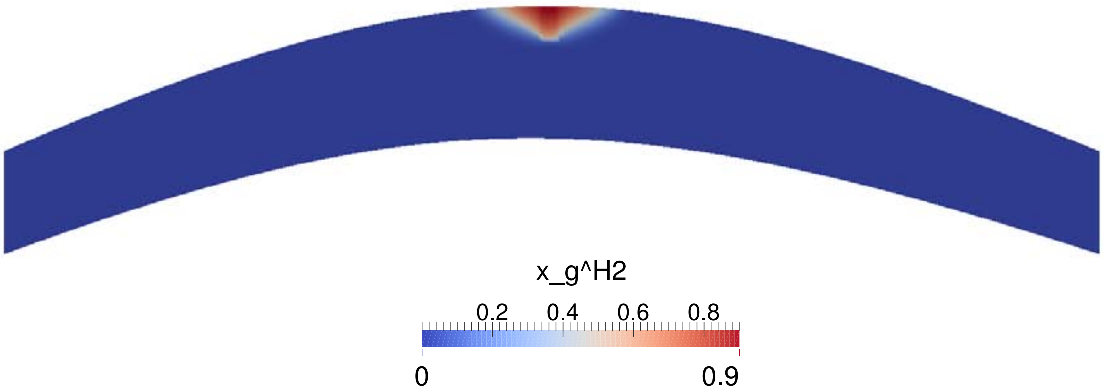
HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

- 2D Geometry: dome-shaped anticline formation
- Initially: Hydrostatic equilibrium, gas composition 20% CO_2 and 80% CH_4, sulfate dissolved in water, presence of methanogenic archaea and sulfate-reducing bacteria
- One well in the top center
- 1 short injection cycle: 50 days hydrogen injection, 100 days idle

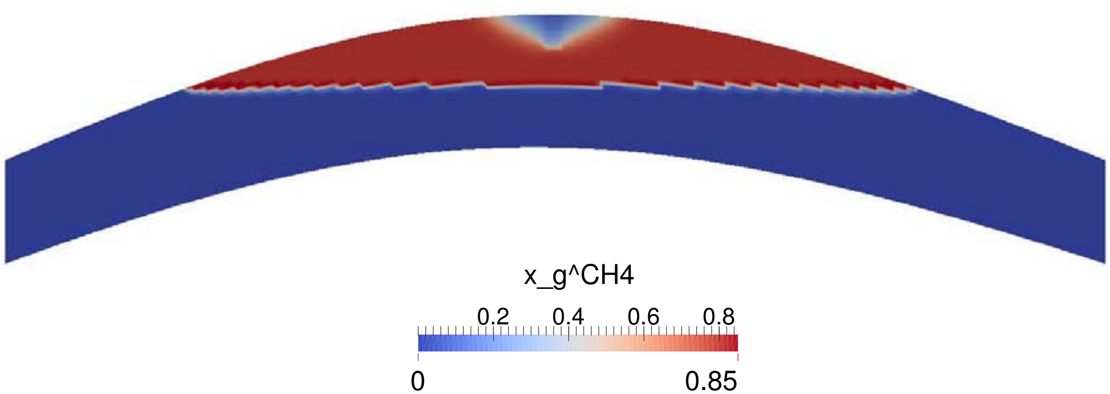


HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

- H_2 concentrations after injection period



- CH_4 concentrations after injection period



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HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

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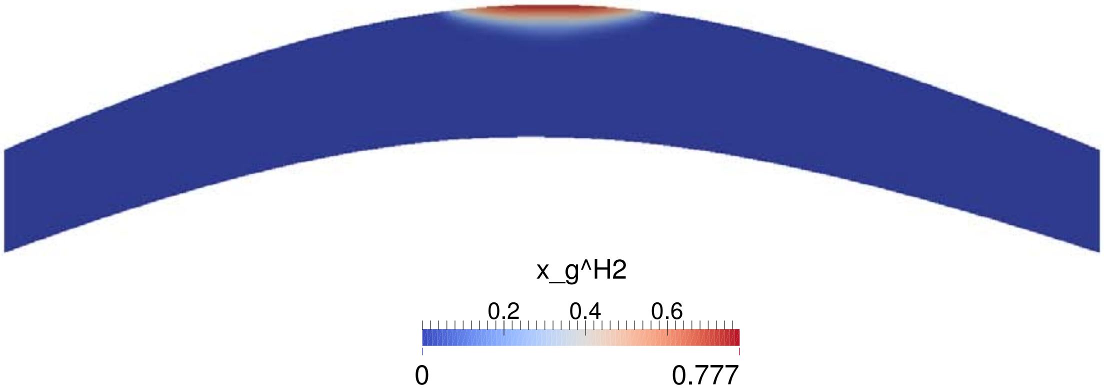

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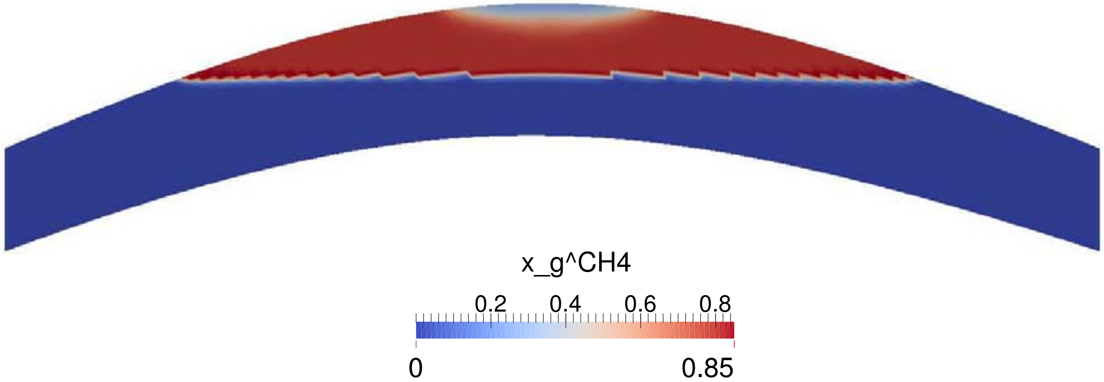
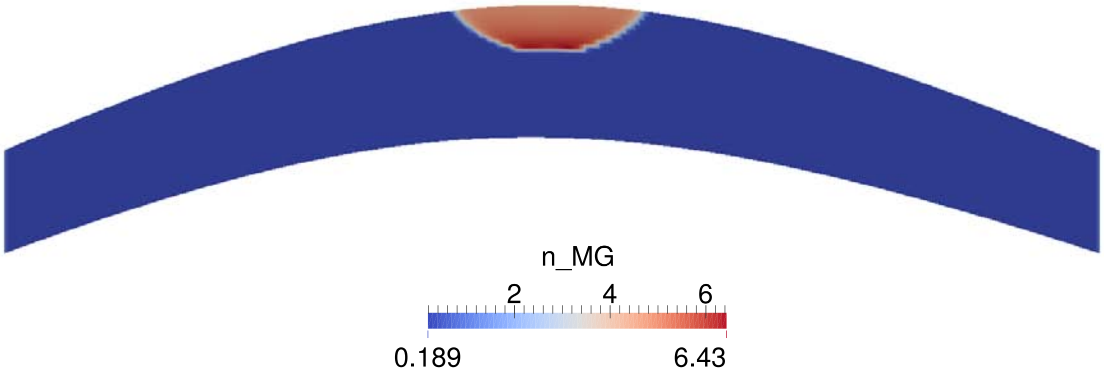
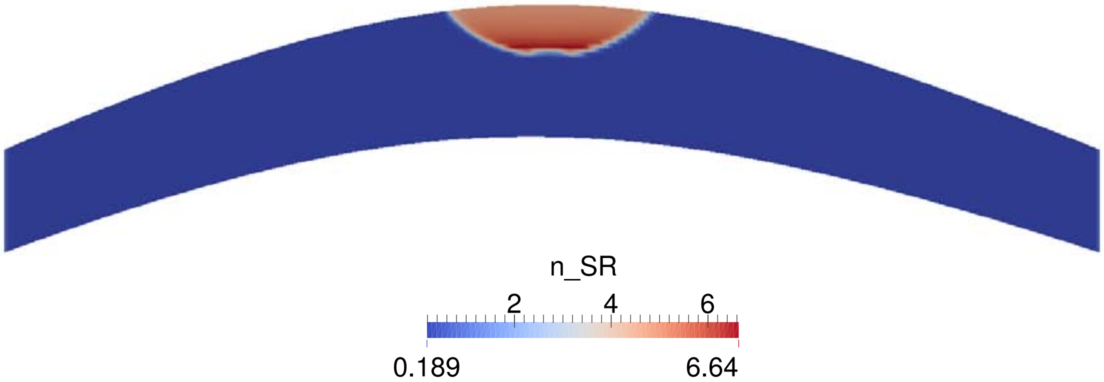


HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

- Number of methanogenic archaea after injection period



- Number of sulfate-reducing bacteria after injection period



HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

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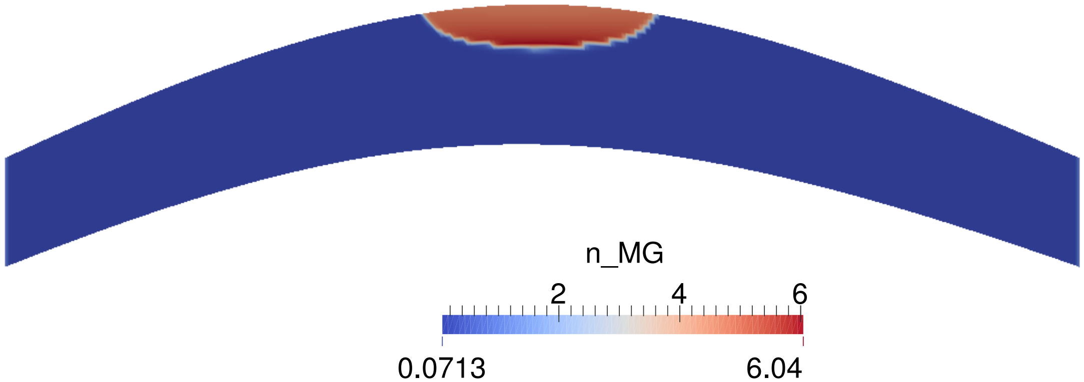

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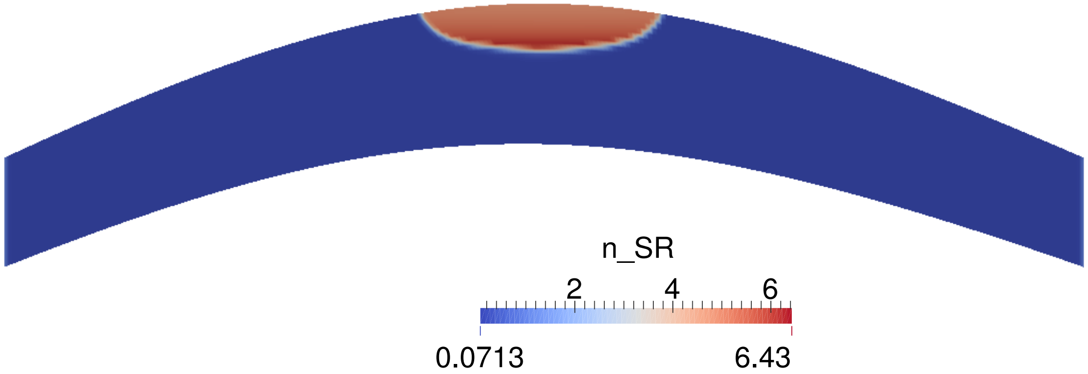
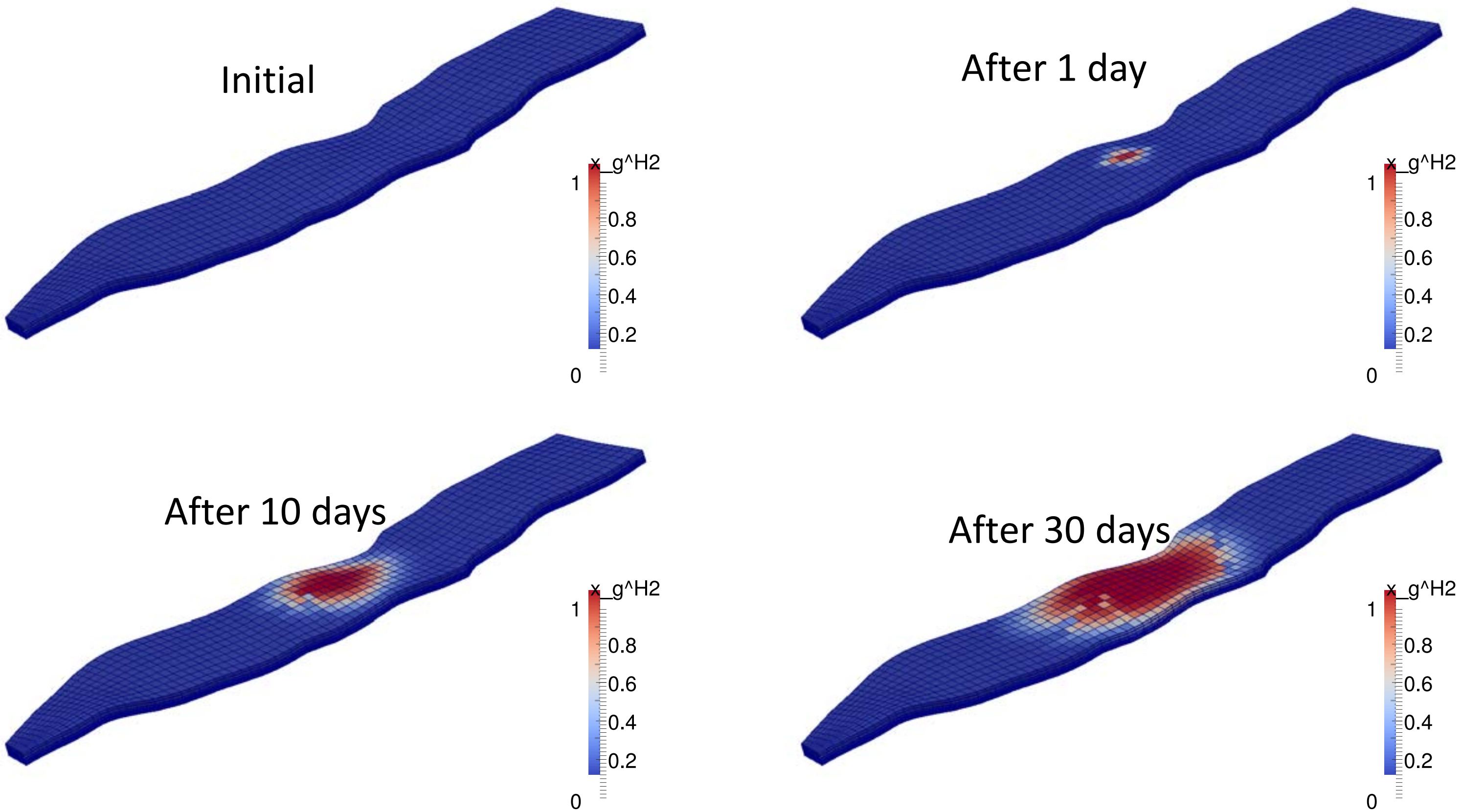


3D SIMULATION USING A REAL GEOLOGICAL MODEL

- H_2 injection by one well



CONCLUSIONS

- A mathematical model was developed and numerically implemented in DuMu^X which describes the coupled hydrodynamic and bio-chemical behavior including multiple microbial species
- Numerical simulations have shown that:
  - A large region of mixed gas (initial and injected) appears in depleted gas reservoirs
  - Lateral fingers appear during fast hydrogen injection in aquifers
  - Hydrogen spreads laterally faster than methane
  - Methanogenesis : Accumulations of microorganisms arise which are accountable for a partial transformation of the injected H_2 into CH_4 and H_2O
  - Sulfate-reduction: Accumulations of sulfate-reducing bacteria arise which produce small amounts of H_2S
  - The kinetic model for microbial growth has an important influence for modeling of bio-chemical reactions
- Only methodical results because the parameters (e.g. for the microbial kinetics) are uncertain

THANK YOU FOR YOUR ATTENTION!