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

- H₂ 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% H₂) 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

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

- **Reactive transport** for 6 mobile components: H\textsubscript{2}, CO\textsubscript{2}, CH\textsubscript{4}, H\textsubscript{2}O, SO\textsubscript{4}\textsuperscript{2-}, H\textsubscript{2}S

\[
\frac{\partial}{\partial t} \left( \rho_g C_g^k S_g + \rho_w C_w^k S_w \right) - \nabla \cdot \left( \rho_g C_g^k \frac{K_{rg}}{\mu_g} \cdot (\nabla P_g - \rho_g g) + \rho_w C_w^k \frac{K_{rw}}{\mu_w} \cdot (\nabla P_w - \rho_w g) \right) \\
- \nabla \cdot \left( \rho_g C_g^k \phi S_g \nabla C_g^k + \rho_w C_w^k \phi S_w \nabla C_w^k \right) = \phi S_w \sum_m \gamma_m \frac{\psi_m^{\text{growth}}}{Y_m} n_m
\]
MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

- Bio-chemical reactions
  - Methanogenesis:
    \[ \text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O} \]
  - Sulfate-reduction:
    \[ \text{SO}_4^{2-} + 5\text{H}_2 \rightarrow \text{H}_2\text{S} + 4\text{H}_2\text{O} \]

- Stoichiometric coefficients

\[
\gamma_M = \begin{pmatrix}
-4 \\
-1 \\
1 \\
2 \\
0 \\
0
\end{pmatrix} \quad \gamma_S = \begin{pmatrix}
-5 \\
0 \\
0 \\
4 \\
-1 \\
1
\end{pmatrix}
\]
MODEL OF BIO-REACTIVE TWO-PHASE TRANSPORT

- Microbial growth functions (Monod model)
  - for methanogenic archaea
    \[
    \psi_M = \psi_{\text{max}} \left( \frac{C_{H_2}^w}{\alpha_{1,M} + C_{H_2}^w} \right) \left( \frac{C_{CO_2}^w}{\alpha_{2,M} + C_{CO_2}^w} \right)
    \]
  - for sulfate-reducing bacteria
    \[
    \psi_S = \psi_{\text{max}} \left( \frac{C_{H_2}^w}{\alpha_{1,S} + C_{H_2}^w} \right) \left( \frac{C_{SO_4^{2-}}^w}{\alpha_{2,S} + C_{SO_4^{2-}}^w} \right)
    \]

- Other growth models were tested
NUMERICAL IMPLEMENTATION
DuMu$^X$ IMPLEMENTATION (2p6c2mo)

- Based on implicit 2p2c model
- New fluids system
  - 2 phases
  - 6 components: H$_2$O, H$_2$, CO$_2$, CH$_4$, SO$_4^{2-}$, H$_2$S (SO$_4^{2-}$ not in thermodynamic equilibrium)
  - 2 microbial species: Methanogenic archaea and sulfate-reducing bacteria
  - Introduction of new components (H$_2$S, 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, bioreaction term added in computeSource(...) (2p6c2molocalresidual.hh)
PROBLEM DEFINITION

- Reservoir initialization \((\text{initialAtPos}(...))\)
  - 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 \((\text{solDependentSource}(...))\)
  - 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% H₂
- 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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HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

- 2D Geometry: dome-shaped anticline formation
- Initially: Hydrostatic equilibrium, gas composition 20% CO₂ and 80% CH₄, 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

- $\text{H}_2$ concentrations after injection period

- $\text{CH}_4$ concentrations after injection period
HYDRODYNAMIC AND BIO-CHEMICAL EFFECTS

- $H_2$ concentrations after idle period

- $CH_4$ concentrations after idle period
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

- Number of methanogenic archaea after idle period

- Number of sulfate-reducing bacteria after idle period
3D SIMULATION USING A REAL GEOLOGICAL MODEL

- $\text{H}_2$ injection by one well

![Initial](image1.png)  
![After 1 day](image2.png)  
![After 10 days](image3.png)  
![After 30 days](image4.png)

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CONCLUSIONS

- A mathematical model was developed and numerically implemented in DuMu\textsuperscript{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 $\text{H}_2$ into $\text{CH}_4$ and $\text{H}_2\text{O}$
  - Sulfate-reduction: Accumulations of sulfate-reducing bacteria arise which produce small amounts of $\text{H}_2\text{S}$
  - 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!