Numerical Study of Biological and Geochemical Reactions during Hydrogen Storage in Subsurface Porous Media

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MY PROFILE

BACKGROUND

- Hydrogen (H_2) is vital in the energy transition as a clean alternative to fossil fuels, requiring **large-scale storage** solutions like Underground Hydrogen Storage (UHS). UHS uses geological formations such as depleted oil and gas reservoirs, salt caverns, and aquifers to store significant amounts of H_2, ensuring supply and demand balance and integrating renewable energy sources effectively.
- The **interplay** between microbial activities and geochemical reactions in UHS is complex and dynamic. Microbial processes like Methanogenesis (**MET**), Acetogenesis (**ACE**), and Sulfate Reduction (**SRB**) use dissolved H_2, affecting the geochemical equilibrium and pH. Geochemical reactions, in turn, influence microbial activity by supplying necessary ions. The reservoir's mineralogy significantly impacts these interactions. Understanding this interdependence is crucial for predicting H_2 loss, byproduct generation, and the long-term impact on storage integrity.

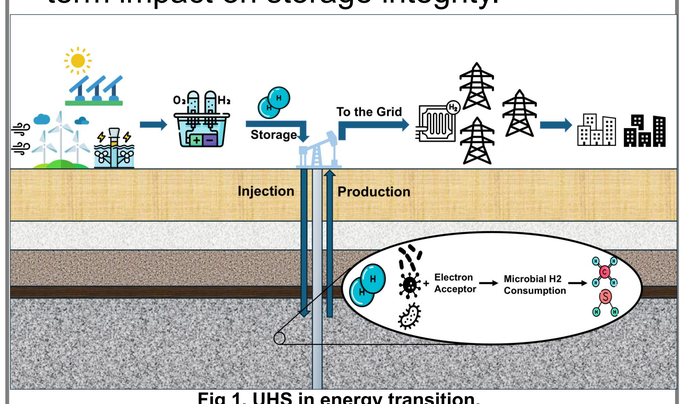


Fig 1. UHS in energy transition.

WHY / PURPOSE

Objectives:

- **Address Bio-Geochemical Knowledge Gaps in UHS.**
- **Develop a Multi-Physics Model for UHS.**

Why?

- ✓ **Hydrogen Loss**
- ✓ **H_2 Purity after Withdrawal**
- ✓ **H_2 Recovery**
- ✓ **Corrosion due to H_2S Formation**

Approach:

- ❑ **Developing a Reactive Transport Model.**
- ❑ **Coupling Bio-Geochemical Reactions with Fluid Flow.**

METHODOLOGY

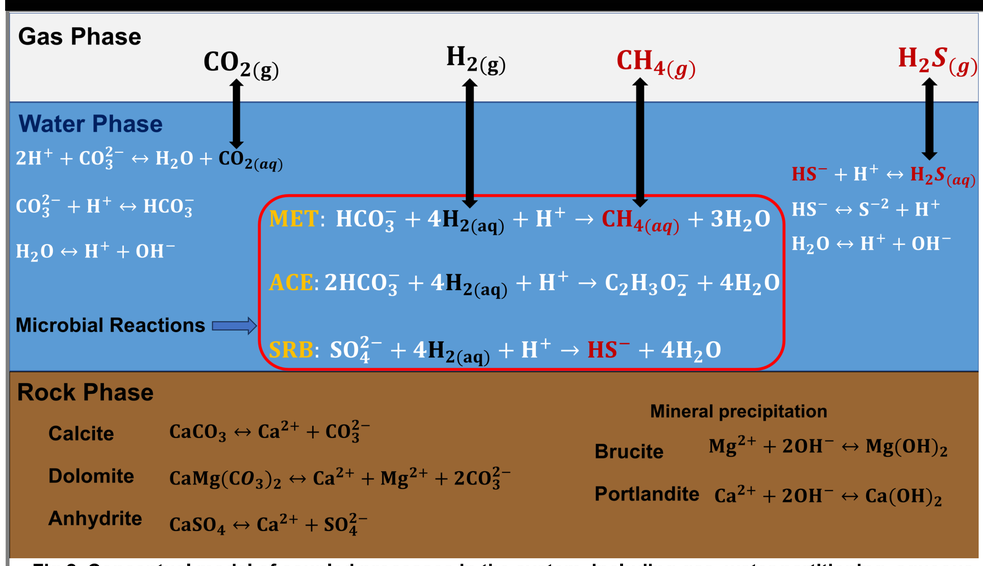


Fig 2. Conceptual model of coupled processes in the system, including gas–water partitioning, aqueous speciation, microbial reactions and rock–water interactions such as mineral dissolution and precipitation.

Batch Model

- **Geochemical Reactions**
  - **Equilibrium**
- **Microbial Reactions**
  - **Kinetic**
  - **Dual Monod Rate Model**
  - $r_S = -\frac{\mu_{max}}{Y}\frac{C_D}{K_D+C_D}\frac{C_A}{K_A+C_A}X$
  - $r_X = -Yr_S - bX$
  - **pH-Temp-Salinity Dependency**
  - $r_{s,corrected} = r_s.\tau(T).\rho(pH).\varepsilon(TDS)$
  - $0 \le \tau(T) \le 1, \tau(T_{opt}) = 1$
  - $0 \le \rho(pH) \le 1, \rho(pH_{opt}) = 1$
  - $0 \le \varepsilon(TDS) \le 1, \varepsilon(TDS_{opt}) = 1$

Microbial Reactions Consume C(4) and S(6)
Rock Dissolution Reactions Provide C(4) and S(6)

→ Microbial Reactions → Equilibrium Disruption → Geochemical Reactions

UHS Dynamics

Reactive Transport Model

MRST TRANSFORMING RESEARCH +

Algorithm

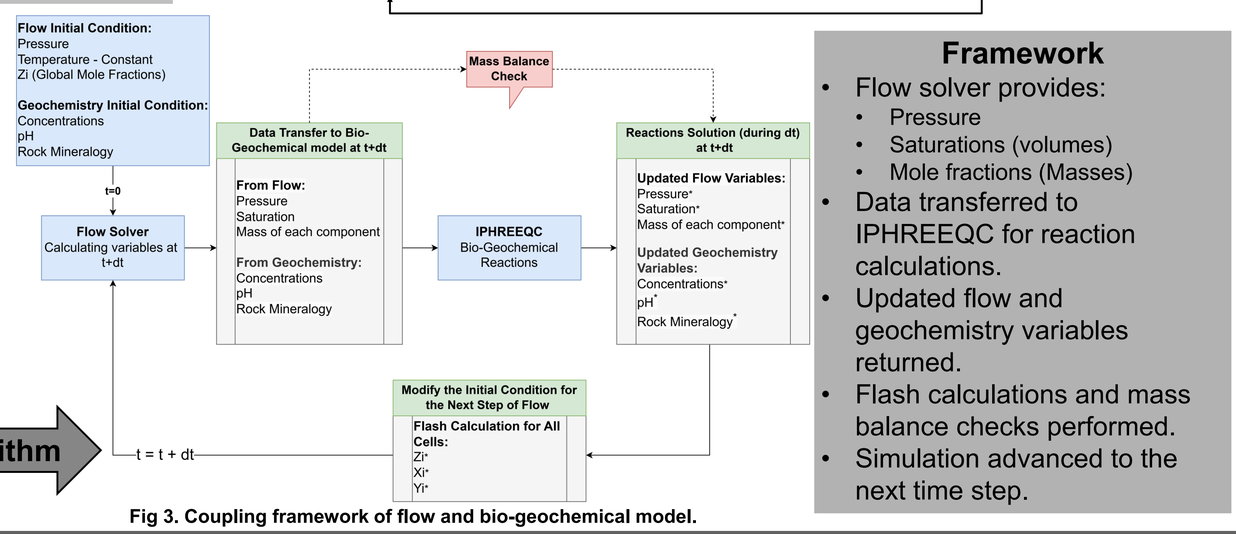
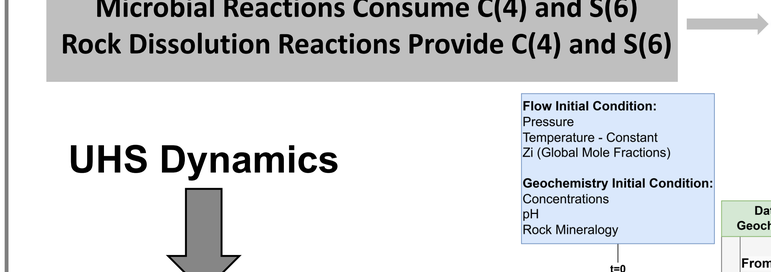


Fig 3. Coupling framework of flow and bio-geochemical model.

Framework

- Flow solver provides:
  - Pressure
  - Saturations (volumes)
  - Mole fractions (Masses)
- Data transferred to IPHREEQC for reaction calculations.
- Updated flow and geochemistry variables returned.
- Flash calculations and mass balance checks performed.
- Simulation advanced to the next time step.

RESULTS



1D Simulation: UHS with Bio-Geo Reactions

Fig 5. y-H2 in three microbial conditions.

Fig 4. Comparison of GEM and our model for pH, Ca^{2+} molality, and $CaCO_3$ dissolution profiles at different pore volumes of injection.

Influence of Reservoir Heterogeneity on Microbial Reaction Dynamics During Underground Hydrogen Storage

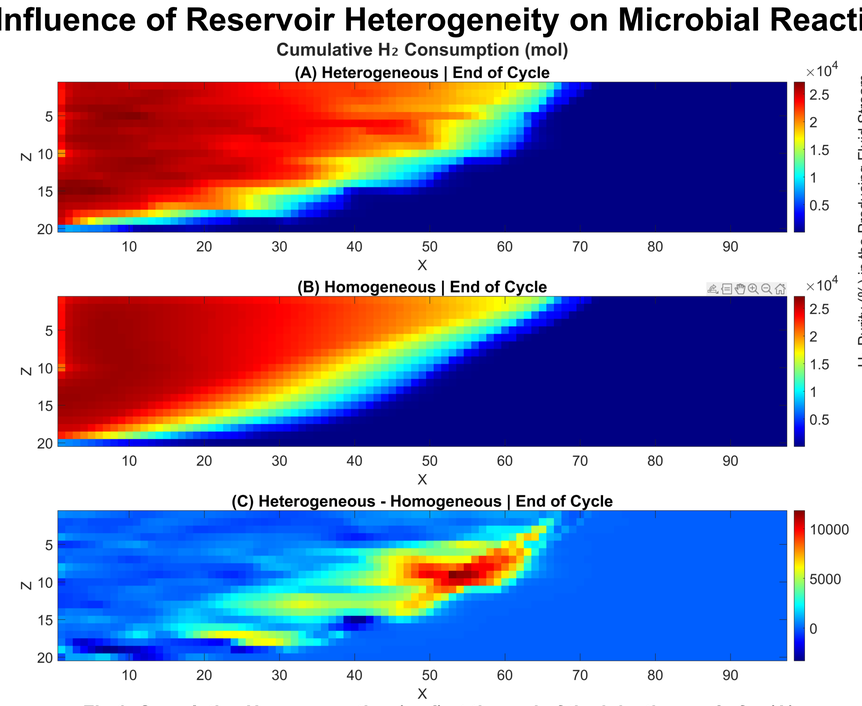


Fig 6. Cumulative H_2 consumption (mol) at the end of the injection cycle for (A) heterogeneous case, (B) homogeneous case, and (C) the difference between heterogeneous and homogeneous systems.

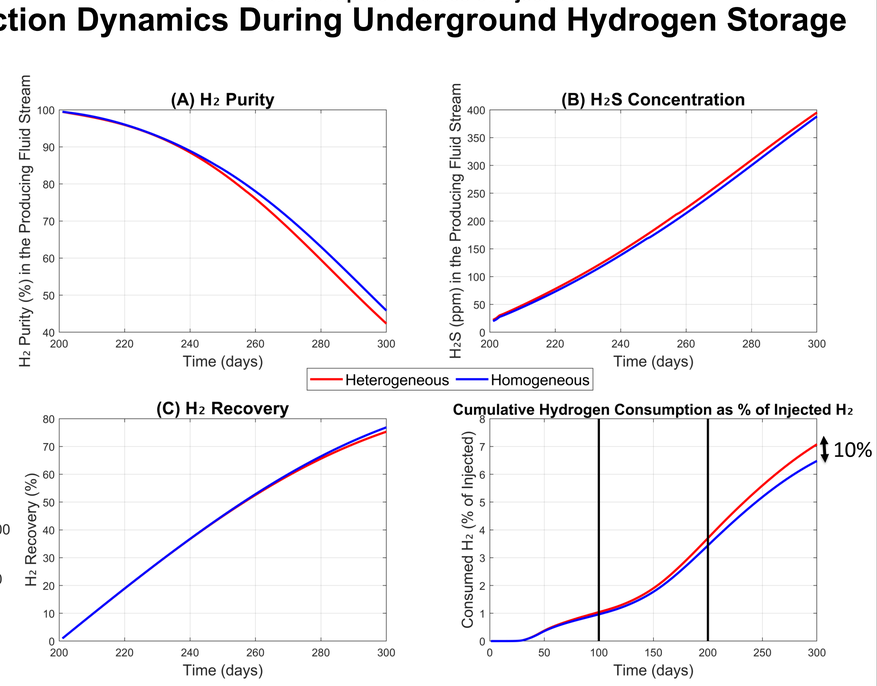


Fig 7. Comparison of heterogeneous and homogeneous cases during back production (days 200–300): (A) H_2 purity, (B) H_2S concentration, (C) cumulative H_2 recovery, and (D) cumulative H_2 consumption in the reservoir (% of injected).

References:

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2- A. Shojaee, S. Ghanbari, G. Wang, E. Mackay., Integrated Modelling of Bio-Geochemical Aspects in Underground Hydrogen Storage: Implications for Reservoir Selection and Performance
3- A. Shojaee, S. Ghanbari, G. Wang, S. Gregory, N. Dopffel E. Mackay., New flow simulation framework for underground hydrogen storage modelling considering microbial and geochemical reactions

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