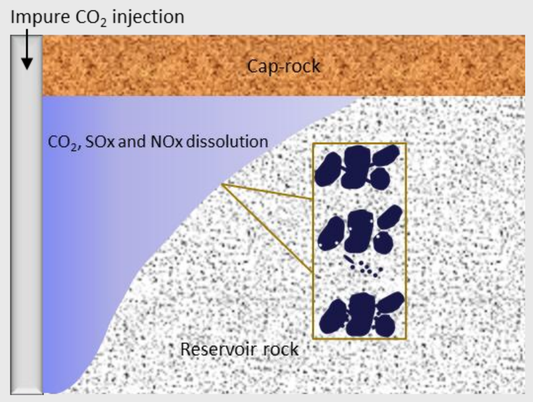
Interactions between impure CO_2 reservoir rock at fluid-formation interface

Ding Xiong, Nicolas Bovet, and Wei Yan

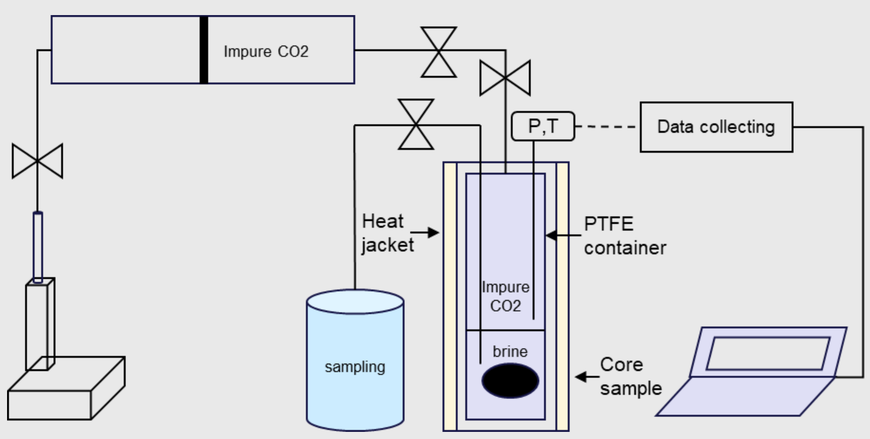
DTU Chemistry
Center for Energy Resources Engineering

Introduction

Carbon capture and storage (CCS) is a critical solution for reducing global CO_2 emissions. While most research focuses on the storage of pure CO_2, industrial emissions often contain trace impurities (e.g., SOx, NOx, amines) that may alter subsurface rock-fluid interactions[1,2]. This study under the MISSION-CCS project investigates the impact of impure CO_2 on reservoir rocks, with **emphasis on near-wellbore chemical processes** during injection.



Experimental Method



1. Baseline build-up (N_2 injection)
2. Impure CO_2 injection
3. Characterizations before and after: SEM, XRD, IC, μ-CT

Simulation Study

Geological modeling → Reservoir simulation → Result analysis

- Geological model from Danish depleted reservoir
- Reservoir properties input in CMG
- Cumstomized impurity (SO_2)
- Chemical reactions coupling
- Numerical control
- Gas composition distribution
- pH evolution
- Porosity development
- Mineral changes

Chemical Reactions

Aqueous reactions

$CO_2 + H_2O = H^+ + HCO_3^-$

$HCO_3^- = H^+ + CO_3^{2-}$

$H_2O = H^+ + OH^-$

$SO_2 + H_2O = H^+ + HSO_3^-$

$HSO_3^- = H^+ + SO_3^{2-}$

Mineral reactions

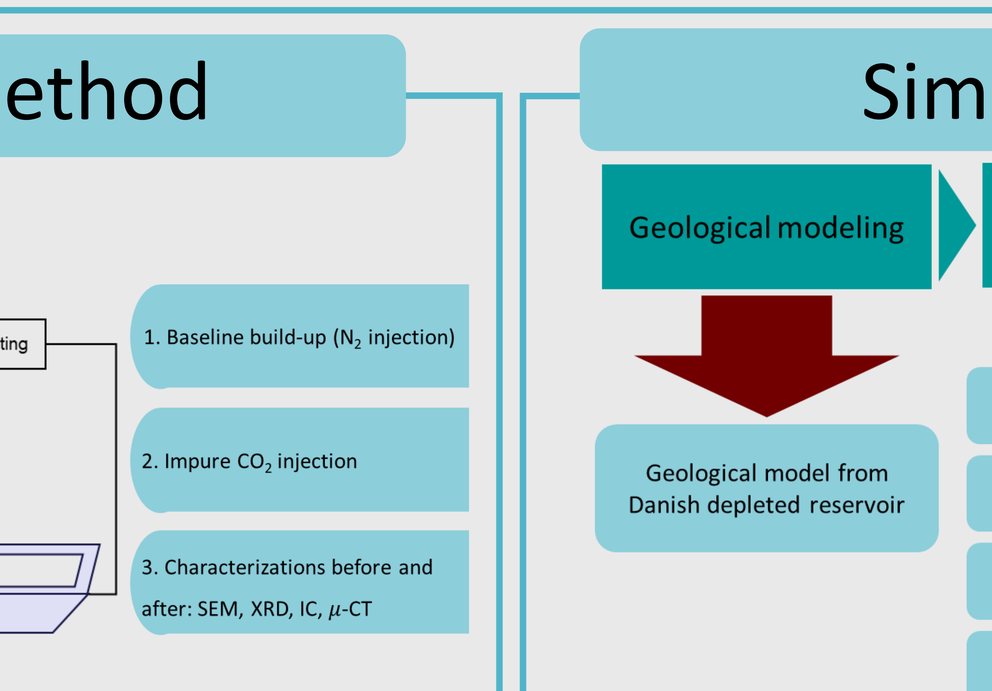
$Gluconite + 7H^+ = 3.75SiO_2 + 0.25Fe^{2+} + 0.5Al^{3+} + 0.75K^+ + 4.5H_2O + 1.25Fe^{3+} + 0.25Mg^{2+}$

$Calcite + H^+ = HCO_3^- + Ca^{2+}$

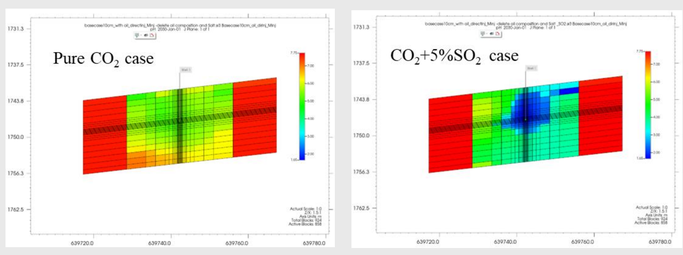
$Siderite + H^+ = HCO_3^- + Fe^{2+}$

$Quartz = SiO_2(aq)$

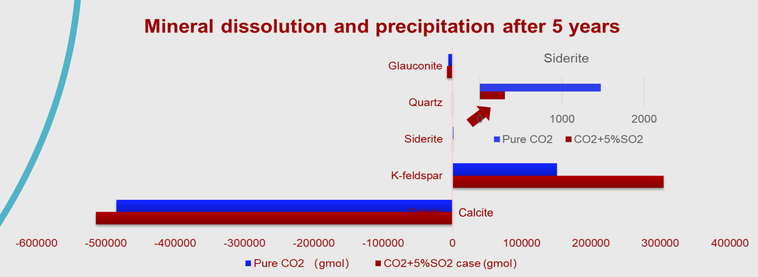
$K\text{-feldspar} + 4H^+ = 3SiO_2 + Al^{3+} + K^+ + 2H_2O$



Simulation results

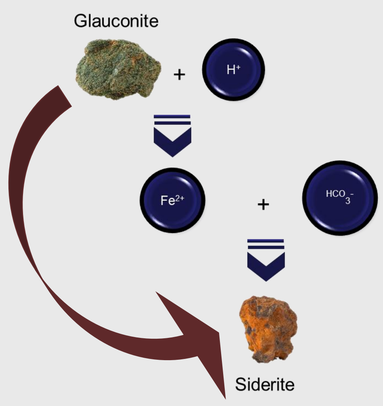


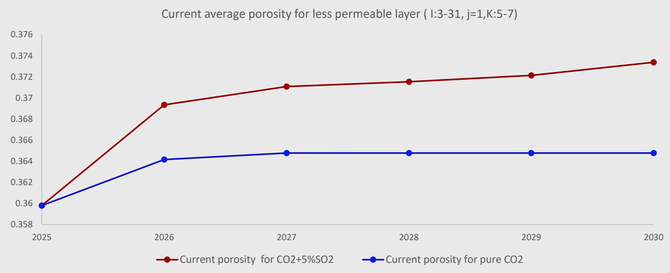
pH evolution for both cases



Mineral composition changes

Key Findings





Porosity development in the selected layers

Conclusions

- **First study** to implement a CMG-based reactive transport model incorporating SO_2.
- CO_2 + 5%SO_2 mixture significantly reduced the **pH (~2)**.
- SO_2 addition amplified dissolution-precipitation asymmetry.
- Identification of **rock conversion from glauconite to siderite**.
- Porosity enhancement of three times higher from SO_2 addition.

Acknowledgements

The authors would like to acknowledge funding provided via the European Commission's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie Grant Agreement ID: 101118369, Material Science Innovation for Accelerated, Sustainable and Safe Implementation of Carbon Capture and Storage (MISSION-CCS),

References

[1] Sonke, J., Morland, B. H., Moulie, G., & Franke, M. S. (2024). Corrosion and chemical reactions in impure CO_2. International Journal of Greenhouse Gas Control, 133, 104075.
[2] Talman, S. (2015). Subsurface geochemical fate and effects of impurities contained in a CO_2 stream injected into a deep saline aquifer: What is known. International Journal of Greenhouse Gas Control, 40, 267–291.