



Contribution ID: 257

Type: **Poster Presentation**

Pore-scale modeling and simulations of microbially induced carbonate precipitation in 3D geologic media through the micro-continuum approach

Wednesday, 21 May 2025 10:05 (1h 30m)

Microbially induced carbonate precipitation (MICP) is a biologically driven mineralization in geologic media, during which the metabolic activity of microorganisms generates urea and further produces CO_3^{2-} , forming calcium carbonate precipitation with free Ca^{2+} . It serves as an emerging eco-friendly technology in areas such as bioremediation, petroleum extraction, and particularly carbon capture, utilization, and storage (CCUS). The MICP processes are highly coupled and complex, and its efficiency is significantly affected by the topology of the geologic media and the environmental conditions in the pore space. A major challenge for modeling MICP in 3D geologic media is the integration of coupled biogeochemical processes into a cohesive set of equations, while also capturing the evolution of porosity and permeability. Recent experimental studies reveal that the 3D topology is critical to control reaction dynamics by redirecting the velocity field, while flow fluctuations affect biomass accumulation, indicating the potential impact on MICP behavior. However, most numerical models simulate MICP in 2D porous geometries and cannot determine the optimal environmental conditions for MICP efficiency.

This study develops a new 3D MICP solver, *micpFOAM*, by using the micro-continuum approach implemented within the OpenFOAM environment. After point-by-point validation against existing experimental and numerical data, the model is applied to simulate 3D MICP processes in various configurations, including a single pore, a beads pack, and a realistic media of quartz sand extracted from XCT scanning. Results show that the effects of secondary flow lead to biomass fluctuations caused by flow instabilities. Structural heterogeneity enhances the secondary flow, further alleviating MICP efficiency. We also evaluate several environmental factors that could improve MICP efficiency. Results show that greater biomass and more homogeneously distributed initial microbial attachment result in higher MICP efficiency. Higher temperatures and pH levels increase MICP efficiency by increasing ureolysis and precipitation rates. However, both rates being high can result in anomalous transport behaviors that reduce MICP efficiency, while a combination of fast precipitation ($K_p = 10^{-2}$) and low ureolysis ($K_u = 10^{-5}$) promote MICP. This model highlights the significant role of secondary flow and environmental factors on MICP behavior, offering an applicable framework for optimizing the MICP efficiency in fields like bioremediation and CCUS.

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References

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Session Classification: Poster

Track Classification: (MS05) Microbial Dynamics in Porous Media: Advances in Biofilms, Biogeochemistry, and Biotechnology