#### InterPore2022



Contribution ID: 214

Type: Oral Presentation

# Upscaling investigations of dissolution using machine learning and GeoChemFoam

Thursday, 2 June 2022 14:45 (15 minutes)

The current conceptual model of mineral dissolution in porous media is comprised of three dissolution patterns (wormhole, compact, and uniform) - or regimes - that develop depending on the relative dominance of flow, molecular diffusion and reaction rate during dissolution. Here, we examine the evolution of pore structure during acid injection using our new fast numerical simulator GeoChemFoam on two synthetic pore spaces of increasing complexity. We examine the boundaries between regimes using transverse dispersion and agglomerative hierarchical clustering and prove the existence of a fourth regime called channelling, where already existing fast flow pathways are preferentially widened by dissolution. Channelling occurs in cases where the distribution in pore throat size results in orders of magnitude differences between transverse, longitudinal dispersion and flow rate for different flow pathways. This focusing of dissolution along only dominant flow paths induces an immediate order of magnitude change in permeability with a comparatively small change in porosity, resulting in a different porosity-permeability relationship than has been previously seen. These new dynamic porosity-permeability relationships are then used to train a machine learning model for predicting permeability change with porosity with local flow and reactive conditions. This model is then bootstrapped to GeoChemFoam's Darcy-Brinkman solver and used to predict dissolution at the Darcy scale. The results are then compared to both traditional upscaling techniques and a full pore-scale simulation. Our results highlight the importance of including pore-scale information in upscaled domains. This work demonstrates that our current conceptual model of dissolution regimes must be modified to include channelling for accurate predictions of dissolution in applications such as geologic carbon storage and geothermal energy production and is the first step in upscaling dissolution for accurate Darcy scale prediction.

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## References

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# Participation

In person

Primary author: MENKE, Hannah (Heriot-Watt University)
Co-authors: GEIGER, Sebastian; MAES, Julien (Heriot-Watt University)
Presenter: MENKE, Hannah (Heriot-Watt University)
Session Classification: MS15

Track Classification: (MS15) Machine Learning and Big Data in Porous Media