Estimation of salt crystallization pressure in a nano-pore: a molecular dynamics simulation study

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Abstract—Salt crystallization in porous media or at their surface is a phenomenon of interest in relation with several important applications, such as soil physics, underground storage of CO₂, civil engineering and the protection of our cultural heritage, to name but a few. Therefore, there is an increasing importance to understanding the processes behind salinization. The growth of salt crystals in confined environments, occurs in many places in the Earth’s surface ans subsurface, from farms to underground water resources. It has been proposed that such crystallization, from a supersaturated fluid, can induce mechanical forces in the solid, which may even lead to permanent damage. In this project, I will try to use molecular dynamics (MD) simulation to study the salt crystallization in a confined pore. I will try to use MD and calculate the capitalization pressure in a clay-brine system.

Keywords—Molecular dynamics simulation; salt capitalization; clay mineral; capitalization pressure

I. INTRODUCTION

When precipitating in confined pores, salt minerals induce a crystallization pressure that may potentially damage the reservoir. The extent of salt damage in porous rocks due to crystallization pressure appears to be largely a function of the solution supersaturation, the interfacial energy of the crystalliquid interface, the localization of precipitation, the growth rate, and the mechanical response of the host rock. A condition for damage to occur is that a crystal continues to grow even in a confined space, thus exerting stress on the rock minerals.

II. METHOD

I use the molecular structure of the Montmorillonite (MMT) clay to represent the pore structure. The chemical composition of the material is 20 Na₀.₇₅[S𝑖₇.₇₅ₐ₁₀.₂₅][A₁₃.₅Mg₅.₅]O₂₀(OH)₄. Water and NaCl molecules will be used as the brine composition with different concentrations. I will use LAMMPS and USC HPC to run the simulations.

III. CONCLUSION

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