



Contribution ID: 627

Type: Oral 20 Minutes

## Anomalous thermal expansion of water in clays

*Tuesday, 15 May 2018 12:11 (15 minutes)*

Under undrained heating, the interstitial water pressure in clays increases two to three times more than what would be expected according to the thermal expansion of bulk water. The thermal pressurization is typically circa 0.5 MPa/K, that is, thermal pressurization can well exceed material resistance upon heating of a few tens of Kelvin, which is critical for many geomechanical applications. The anomalous thermal expansion of confined water is also observed for other materials, notably silica and cement. In this study, we investigate this phenomenon by molecular simulation and confront the case of water in a model of montmorillonite to that of a Lennard-Jones fluid in a slit pore. The results show that the thermo-mechanical properties (thermal rigidity and thermal expansion) of the two confined fluids follow similar evolutions both in function of temperature and in function of bulk fluid pressure. In contrast, the bulk fluids have quite different evolutions since water is well known to exhibit negative thermal expansion below 4°C. Accordingly, these results tend to show that the anomalous thermal expansion of confined water is rather due to the anomalous behavior of bulk water. The physical origin of the low temperature behavior of water is generally attributed to the hydrogen bond network. Since this network is highly perturbed in the confined space, this could explain why confined water does exhibit a 'normal' behavior.

### References

### Acceptance of Terms and Conditions

[Click here to agree](#)

**Primary authors:** BROCHARD, Laurent; HONORIO, Tulio (Université Paris-Est Créteil, Laboratoire MSME)

**Presenter:** BROCHARD, Laurent

**Session Classification:** Parallel 4-E

**Track Classification:** MS 1.12: Fluids in Nanoporous Media