Thermo-Hydro-Mechanical Properties of Water-Saturated Clay as a Function of Dry Density and Temperature

Xiaojin Zheng and Ian C. Bourg

Department of Civil and Environmental Engineering, Princeton University

xiaojin.zheng@princeton.edu

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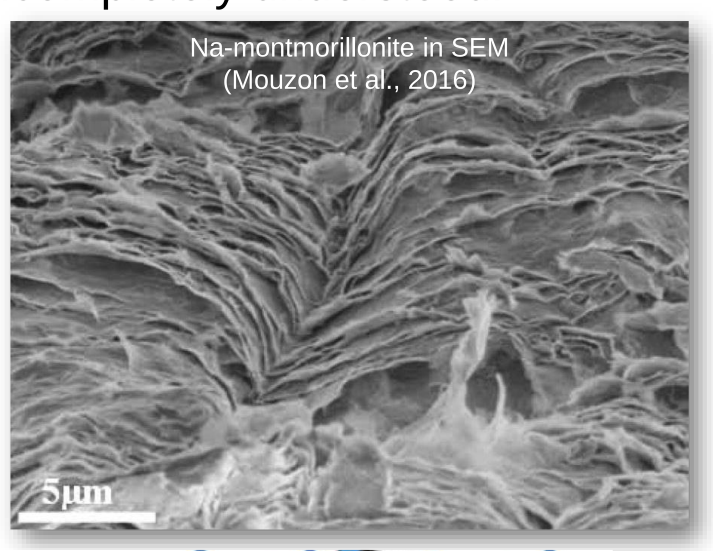
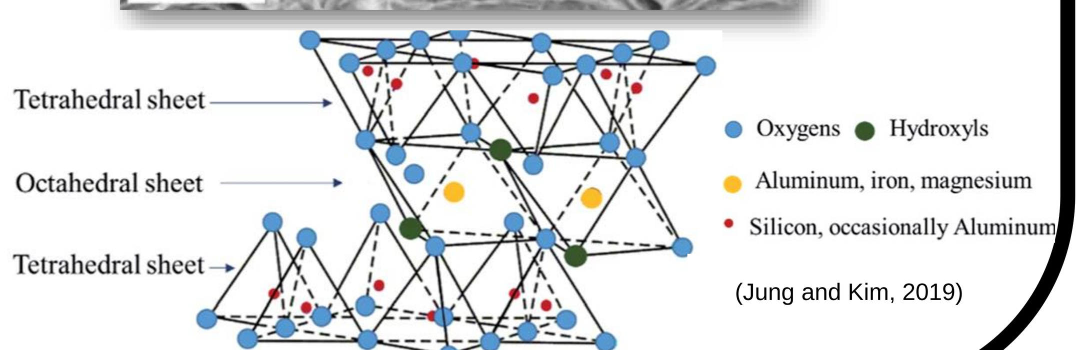
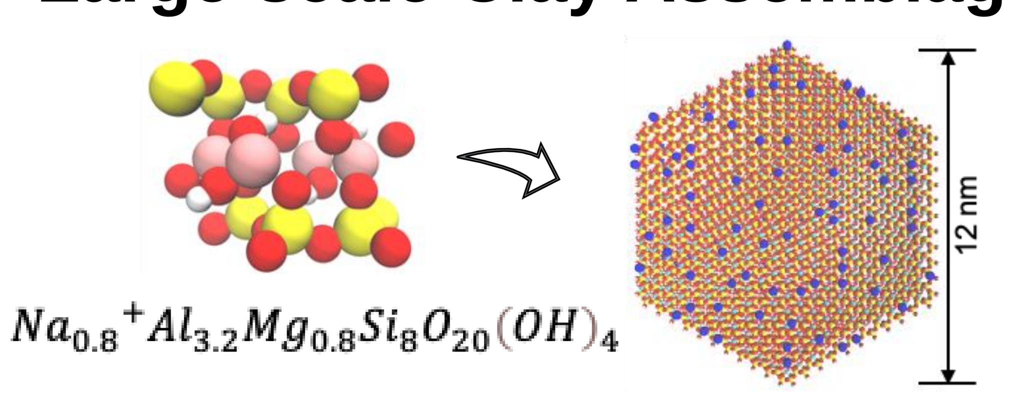
Introduction

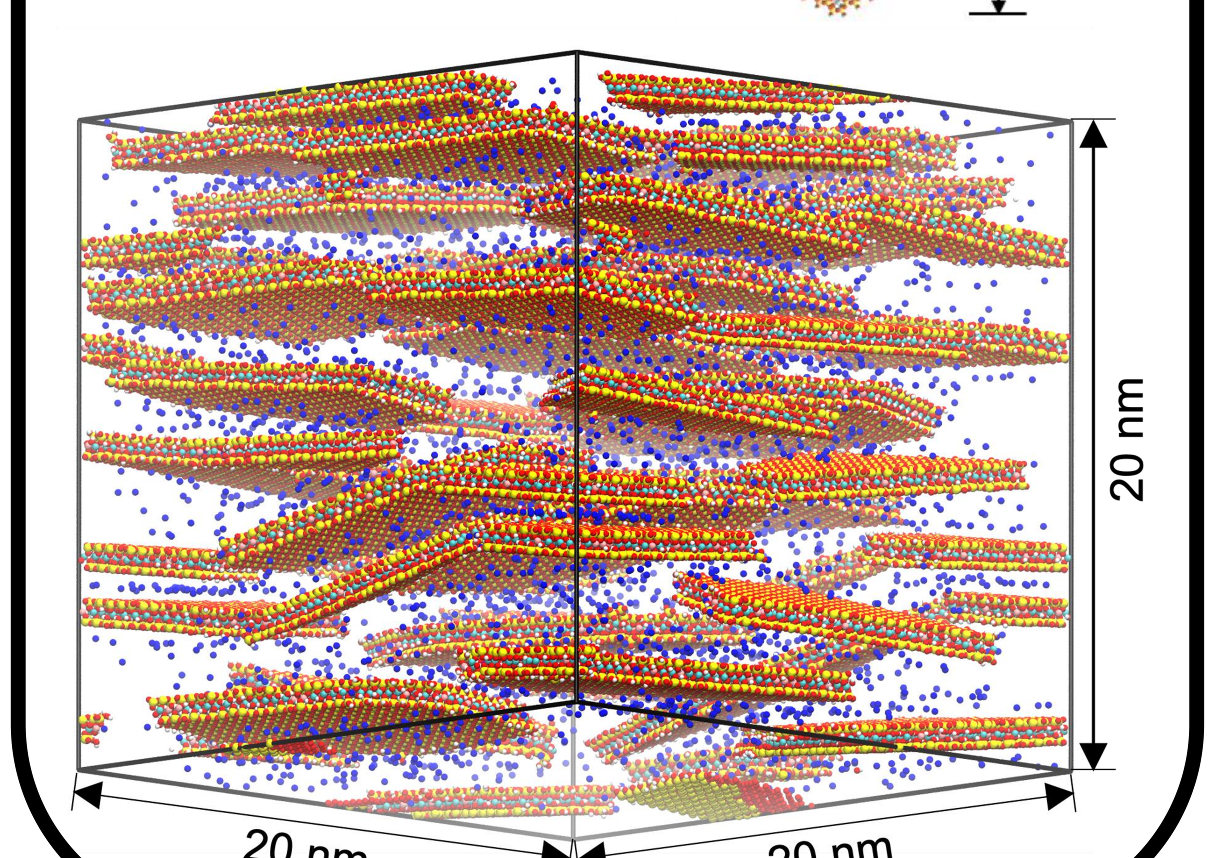
Bentonite is a fine-grained geologic material consisting mainly of montmorillonite clay. It is an important component in current efforts to design engineered barrier systems for the isolation of radioactive waste. However, constitutive relations characterizing the thermal-hydrologic-mechanical-chemical (THMC) coupled properties of bentonite in variable temperature and dry density conditions remain incompletely understood.



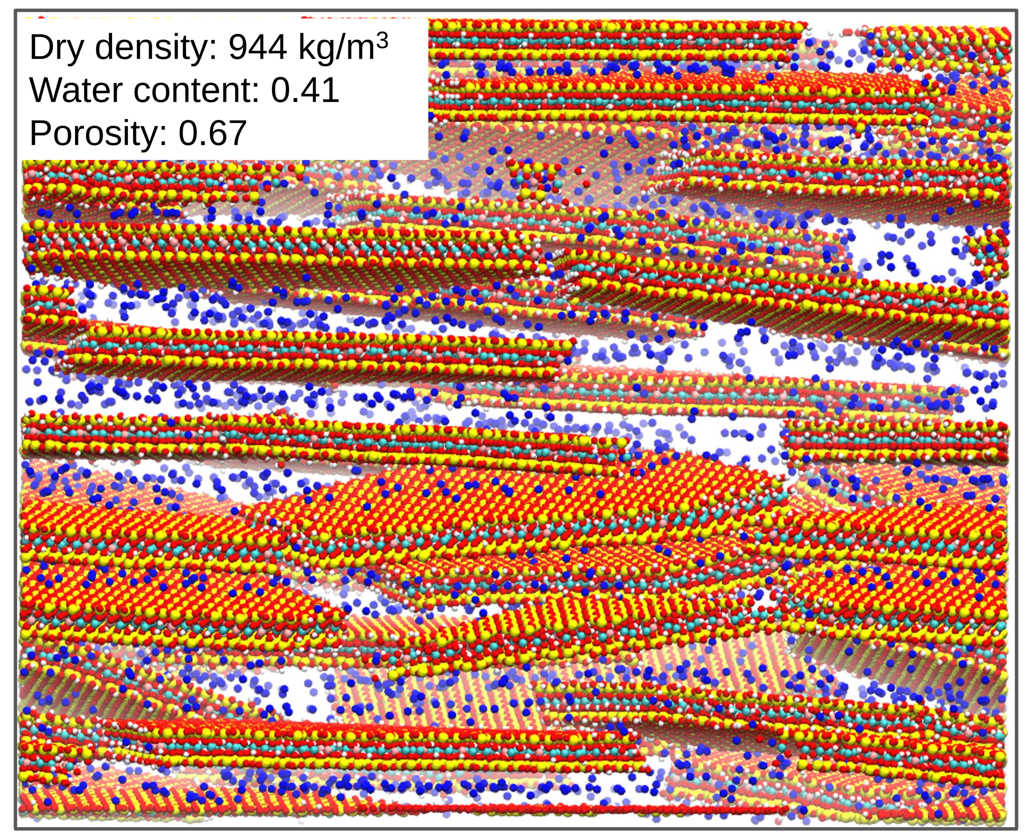


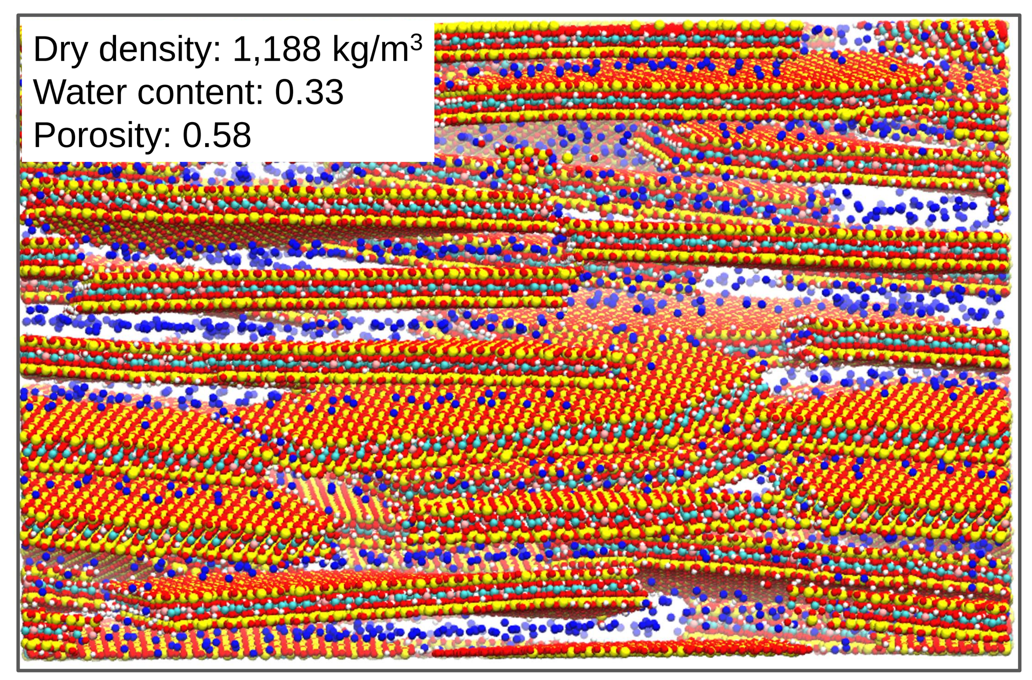
Replica Exchange Molecular Dynamics (REMD) Simulations on Large-scale Clay Assemblages

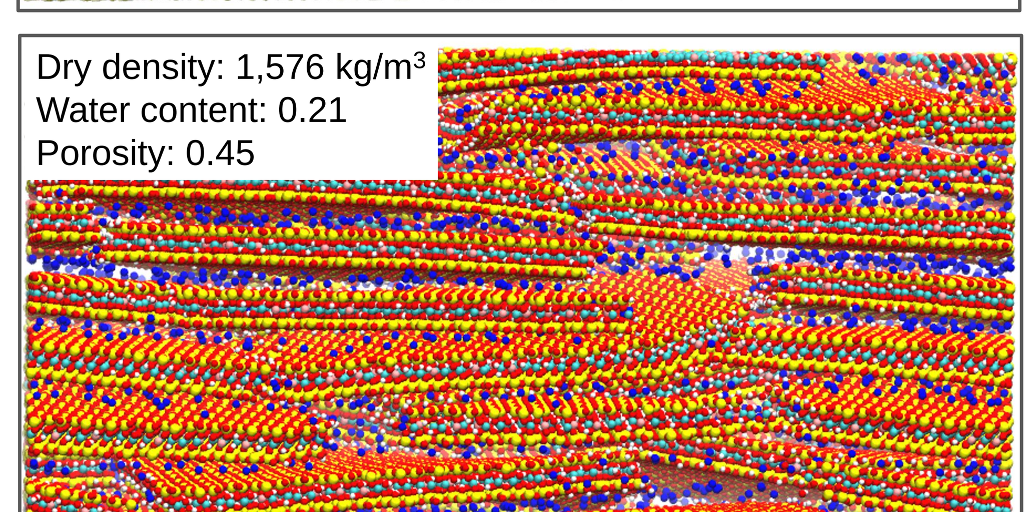




Progressive Dehydration







Simulation Analyses

Heat capacity

$$C_V = k_B \int_0^{\infty} \begin{bmatrix} DoS_{gas}(v) W_{gas}^{c_V}(v) \\ + DoS_{solid}(v) W_{solid}^{c_V}(v) \end{bmatrix} dv$$

$$C_P = C_V + VT \frac{\alpha_P^2}{\kappa_T}$$

Thermal conductivity

$$\lambda = \frac{1}{3Vk_BT^2} \int_0^{\infty} \langle \boldsymbol{J}(t) \cdot \boldsymbol{J}(0) \rangle \, dt$$

Thermal expansion coefficient

$$\alpha_P = \frac{\langle \delta V \delta(\mathcal{H} + PV) \rangle_{NPT}}{k_B T^2 V}$$

Hydraulic conductivity

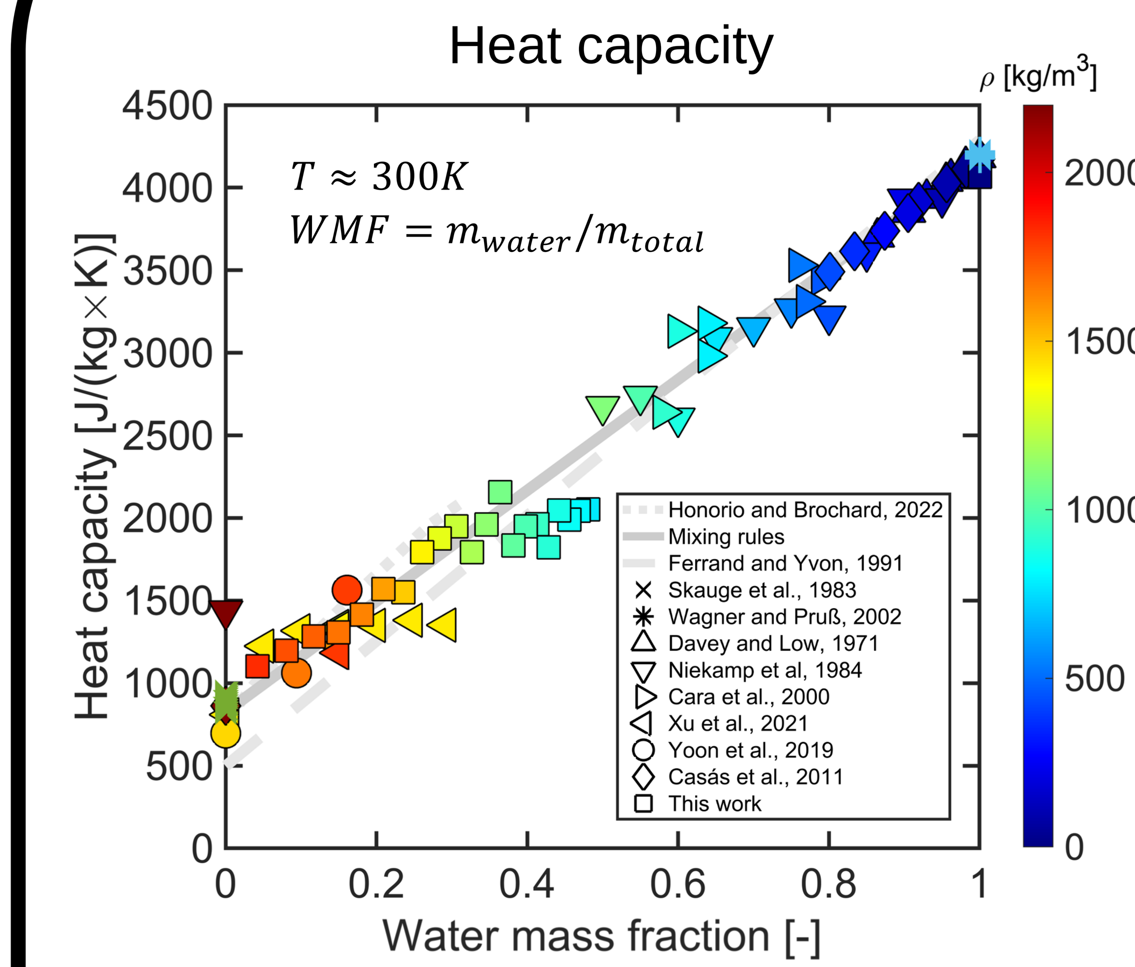
$$k = \frac{\mu V}{k_B T} \int_0^{\infty} \langle v(t) v(0) \rangle dt$$

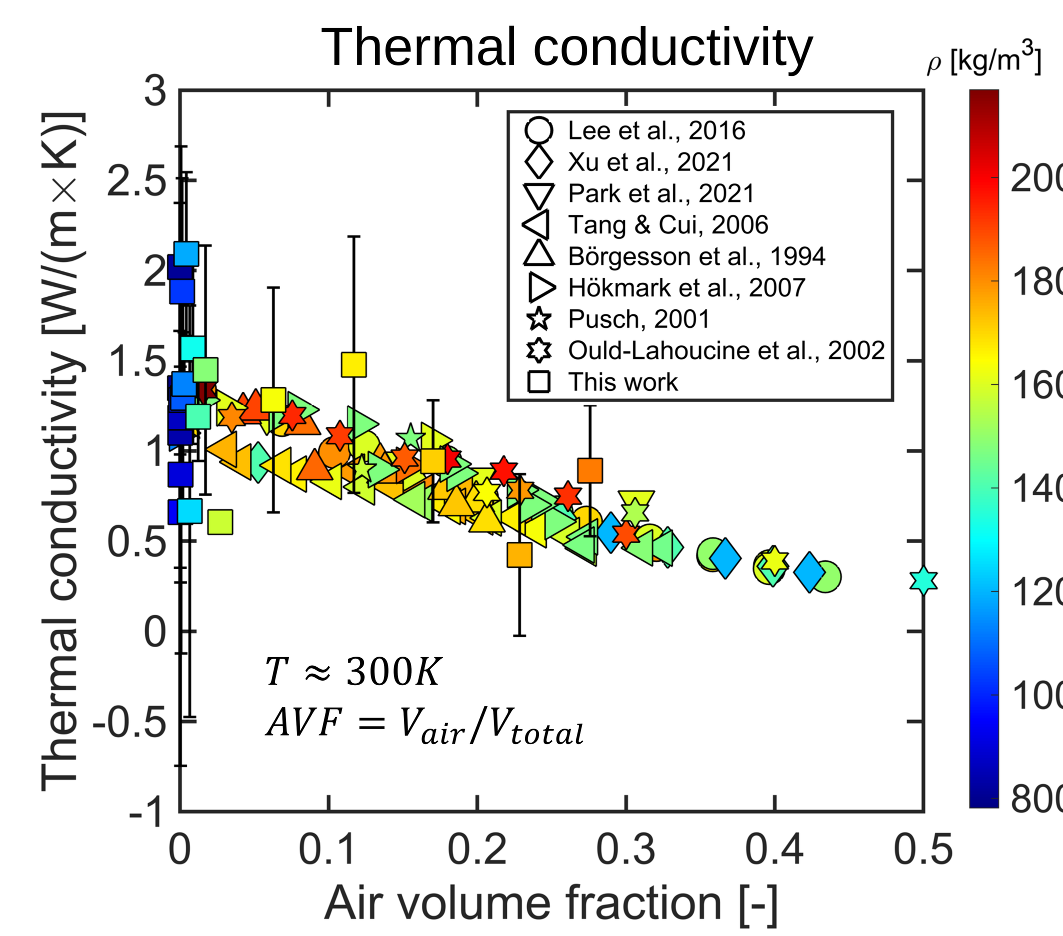
$$K_{cond} = k\rho g/\mu$$

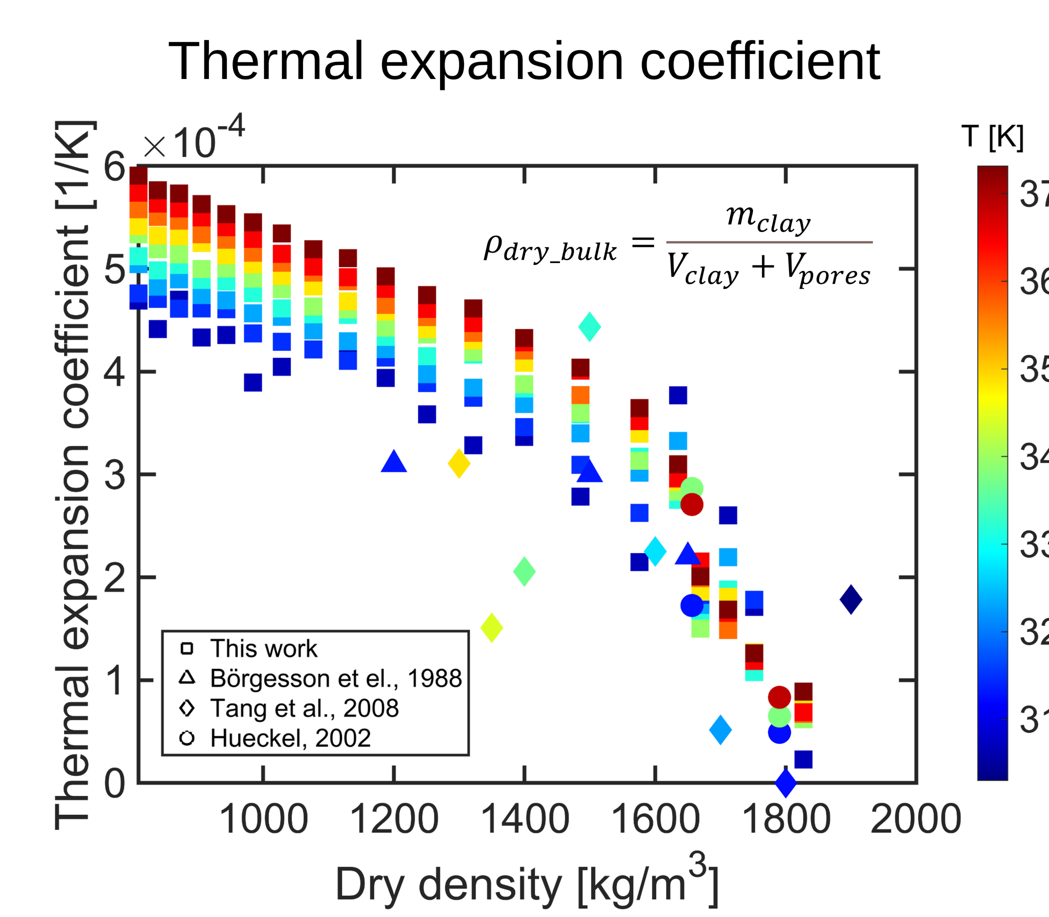
Diffusion coefficient

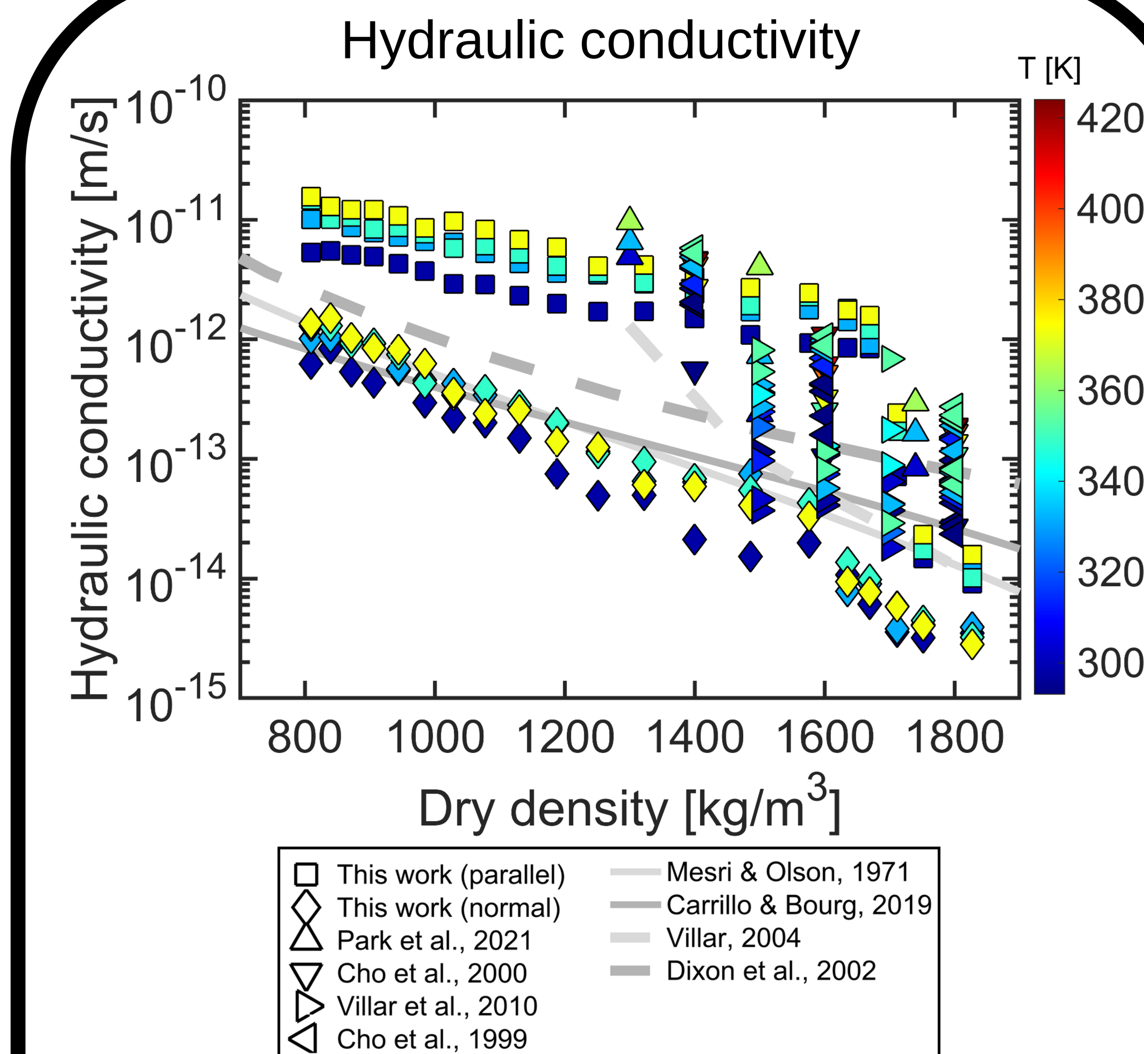
$$D = \frac{1}{2d} \lim_{t \to \infty} \frac{\frac{1}{N} \sum_{i=1}^{N} \left(r_i(t) - r_i(0)\right)^2}{t}$$

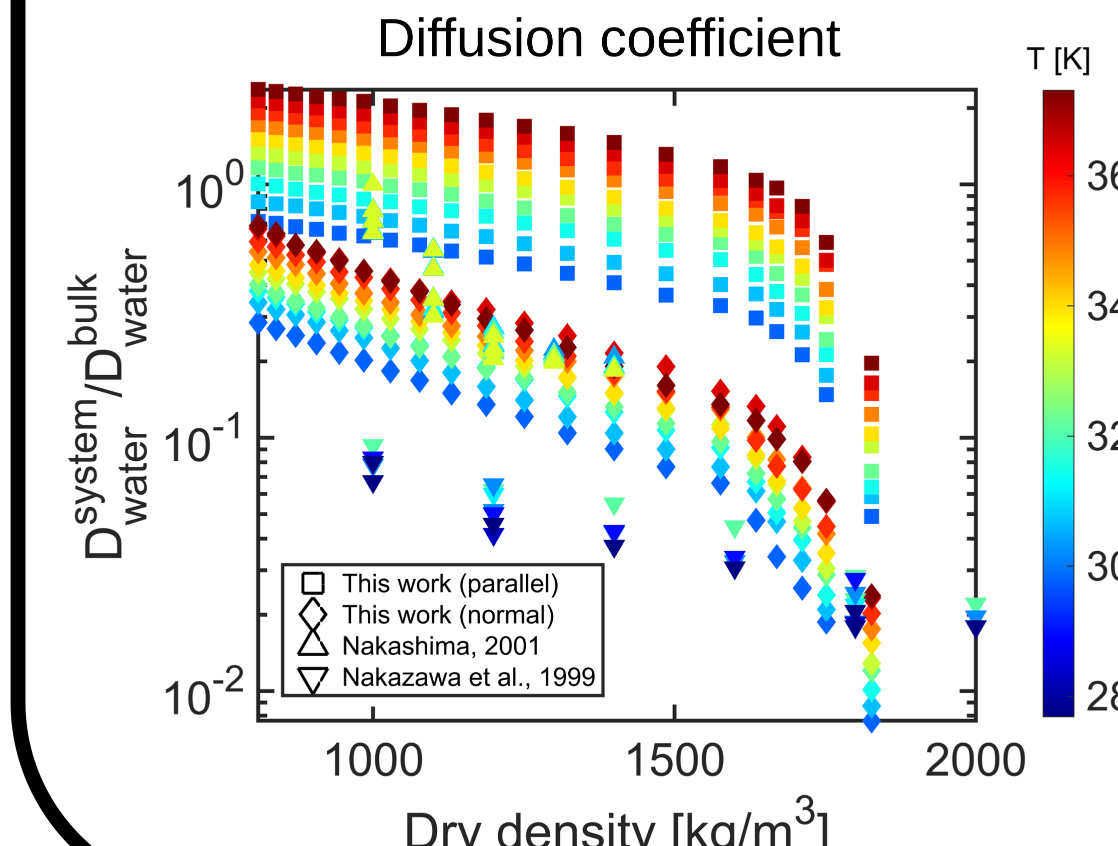
Results











Concluding Remarks and Acknowledgments

- The water content dictates the heat capacity of bentonite.
- The air volume fraction plays a critical role in determining the thermal conductivity of bentonite.
- Low dry bulk density and high temperature enhance the thermal expansion of bentonite.
- Hydraulic conductivity and water self-diffusivity are highly sensitive to orientation, temperature, and dry density.

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