



Contribution ID: 764

Type: Oral Presentation

Molecular Dynamics Simulations of Porous Illite Clay Surfaces and Particles

Monday, 13 May 2024 13:55 (15 minutes)

Illite clay constitutes the main component of the Norwegian quick clay that is known for its tendency to transform rapidly from a solid to a liquid state under certain pressure.¹ Currently the practical method for stabilizing quick clay involves the use of cement and lime, resulting in significant CO₂ emissions.² To explore more environmentally friendly stabilizers, nanoscale theoretical understanding of the mechanical forces between illite particles is essential. The interaction between clay particles depends on the thickness of electrical double layer (EDL) that can be controlled by the types and concentrations of salts.³ In quick clay, a higher salt content results in a thinner EDL and reduced repulsive force. Conversely, if the salt is leached out due to underground water, the EDL thickens, leading to a stronger repulsive force and worse stability. This research primarily focuses on non-equilibrium molecular dynamics simulations involving the direct contact between an illite particle and surface. It aims to elucidate the connections between this interaction and the variations in the EDL resulting from the addition of different salts, such as NaCl, KCl, CsCl, and CaCl₂.

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References

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Session Classification: MS04

Track Classification: (MS04) Swelling and shrinking porous media