A molecular dynamics study about water adsorption in expansive clays

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Introduction: With the increased use of dredged materials for building, it has become more important to understand clay mineral behaviour and its impact on sediment strength and stability. Field and laboratory studies have demonstrated that cohesive sediment stability is strongly influenced by numerous properties of the inorganic and organic fractions and water chemistry [1]. However, conflicting findings highlight the need for a physics-based representation of cohesive sediment stability to understand the atomic interactions[2]. The aim of this study is to use molecular dynamics models to investigate how clay minerology interacts with salinity to affect water absorption (i.e. swelling) and clay structure.

Methods: A molecular dynamics model was created of clay minerals and water using LAMMPS to simulate the hydration behavior of clay particles. The interaction between the atoms were provided by SPC water model[3] and CLAYFF forcefield[4]. A multifactorial design was used with three factors: mineralogy, total salinity, sodium adsorption ratio. For clay mineralogy, kaolinite, beidellite and montmorillonite (MMT) of three interlayer cations were tested - potassium (K-MMT), sodium (Na-MMT) and calcium (Ca-MMT). MMT are expansive clay minerals consist of numerous individual layers stacked together, whereas the individual layer consists of an octahedral (O-) layer sandwiched between two tetrahedral (T-) layer (Figure 1). The clay particle in contact with bulk water were simulated for 2 ns in the isobaric-isothermal (NPT) ensemble, with constant temperature (300 K) and pressure (1 bar). The change of interlayer distance *d* (i.e., the average distance between the bottom silicon atoms of the upper layer and top silicon atoms in the lower layer) was analysed.

Results: Preliminary results show distinct swelling behavior of K-MMT, Na-MMT and Ca-MMT in hydration (Figure 2). Interlayer distance is unchanged for K-MMT but increases by 3-4 fold for Na-MMT and Ca-MMT. Notably, Ca-MMT swells at a much faster rate than Na-MMT.

Discussion: Modelled results agree well with prior observations, providing additional detail and an atomic-level understanding of swelling behavior. K-MMT (Na/Ca-MMT) is known as non-swelling (swelling) clay, thus the constant d is expected. The differences between Na-MMT and Ca-MMT highlight the importance of hydration energy of the cations, i.e., K<Na<Ca. These results illustrate the importance of interactions between sediment and water properties that affect the structure and stability of cohesive sediment and their potential reuse for construction.

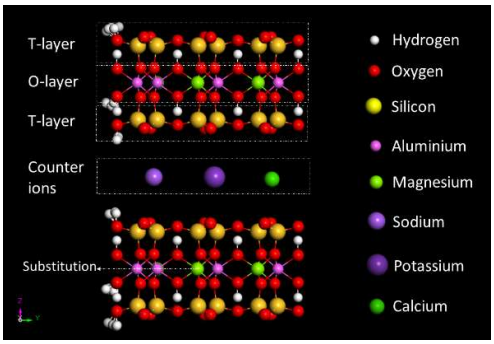

Fig. 1: The MMT sample consists of 42 unit cell ($Al_4Si_8O_{20}(OH)_4$), with 32 Al in the O-layer replaced by Mg, and 32/16 K(Na)/Ca in the interlayer space.

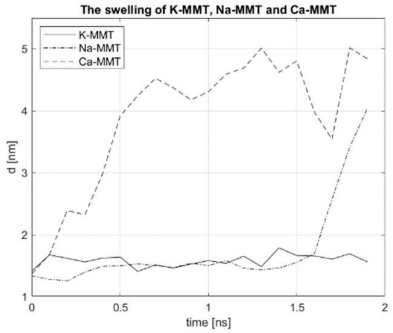

Fig. 2: The evolution of interlayer distance *d*.

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