EGU22-1172
https://doi.org/10.5194/egusphere-egu22-1172
EGU General Assembly 2022
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Modelling short-range interaction of clay particles to improve erodibility prediction

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Introduction: Erosion has become an urgent problem to society due to the increasing intensity and frequency of disturbances, e.g. storms, wave energy and rainfall. Yet, a universal model to predict erosion thresholds for cohesive sediment is still missing. Short range interaction of clays is recognized as the source of cohesion and adhesion of cohesive sediment. The interaction of negatively charged (i.e., montmorillonite (MMT) and beidellite (BD)) and neutral clay particles (i.e., kaolinite (KL)) are traditionally simulated through DLVO theory and van der Waals interaction[1]. However, the applicability of DLVO theory at short range (i.e., at distance less than 3 nm) has been increasingly challenged in molecular dynamics simulations[2]. A suitable description of short-range clay particle interaction is crucial for the prediction of cohesive sediment erodibility. The aim of this study was to determine how clay mineralogy and water chemistry influence clay particle interactions at short range to affect inter-particle attraction and stability under imposed forces.

Methods: Molecular dynamics models of clay minerals and water were created using LAMMPS to simulate the interactions between water, clay and dissolved salt to investigate the forces determining clay cohesion, i.e. attractive force between clay particles [3]. A 2-layer model was used in this study, which is a simplification of the multi-layer particles found in nature. A multifactorial design was used with two factors: mineralogy and salinity. For clay mineralogy, kaolinite (KL), beidellite (BD) and montmorillonite (MMT) with sodium (Na) counter ions were tested. Three types of salt were considered, i.e., KCl, NaCl and CaCl2, with concentration ranging from 1% to 4%. Clay particle interactions with bulk water containing salt solution were simulated for 5 ns. Clay swell, i.e. the increase in the interlayer distance (d the distance between the mass center of two adjacent layers) and the underlying forces were quantified. The resistance of clay particles to imposed force was also investigated.

Results and Discussion: First, for most negatively charged MMT and BD treatments, positively charged cations act as a bridge to hold clay layers together, which contrasts with the swelling predicted by DLVO theory. Second, Na-MMT with -0.375, -0.5, and -0.625 e/unit swelled in pure water, induced by the breakdown of cation bridges rather than osmotic swell pressure. Third, low concentrations of dissolved salt (i.e. KCl, NaCl or CaCl2) inhibit the swelling of MMT, by increasing

the cation bridge strength. Fourth, non-charged KL did not swell because of strong van der Waals interaction. Finally, stable clay particles were more resistant to external pull and shear forces. These novel molecular dynamics simulations are helping to uncover the mechanisms controlling clay cohesion to support new formulations to predict the erodibility of cohesive sediment.

Acknowledgements: The support of the UK Engineering and Physical Sciences Research Council (EPSRC) under grant EP/T001100/1.

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2022-05-27
EGU: European Geophysical Union
https://doi.org/10.5194/egusphere-egu22-1172
Chen W, Grabowski R, Goel S. (2022) Modelling short-range interaction of clay particles to improve erodibility prediction. In: EGU General Assembly, 2022, 23-27 May 2022, Vienna, Austria. Paper number EGU22-1172

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