Wettability of Kaolinite Surfaces with a Water-Cyclohexane Mixture: A Molecular Dynamics Study

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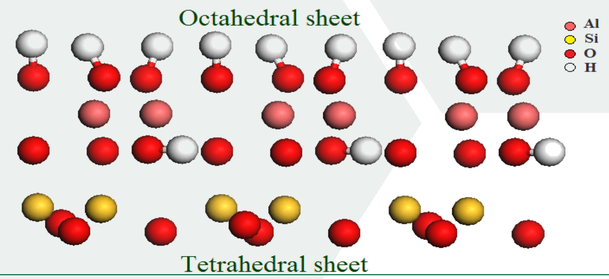
BACKGROUND

- Solvent-based bitumen extraction: an environmentally-friendly alternate to the conventional water extraction
- Environmental and financial urge for recovery of the solvent to levels lower than 290 mg/kg
- Atomistic-level simulations: a powerful tool for inspecting the solvent's behavior in the porous structure of the clay mineral, and examining the role of different parameters which impact its retainment

AIMS AND OBJECTIVES

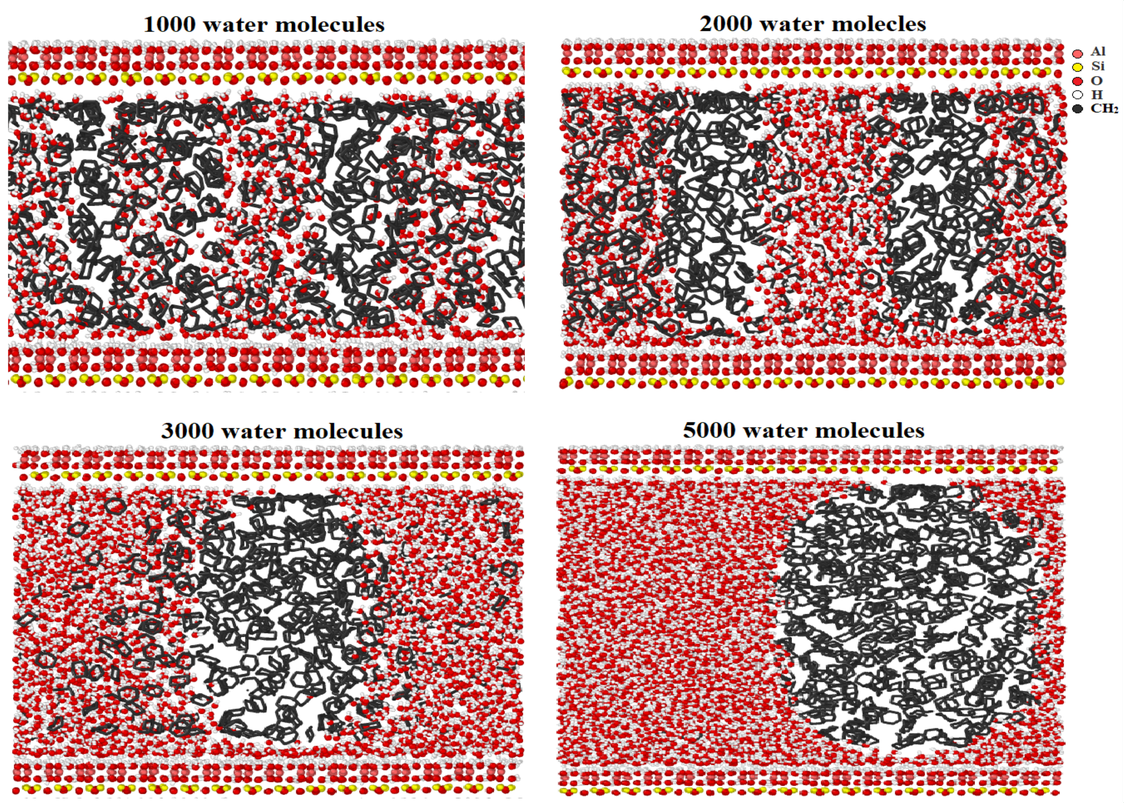
- Investigating wettability of the octahedral and tetrahedral basal surfaces of kaolinite in the presence of an oil phase (cyclohexane)
- Examining the effect of salt on the phase behavior of water and cyclohexane within a kaolinite nano-pore



RESULTS

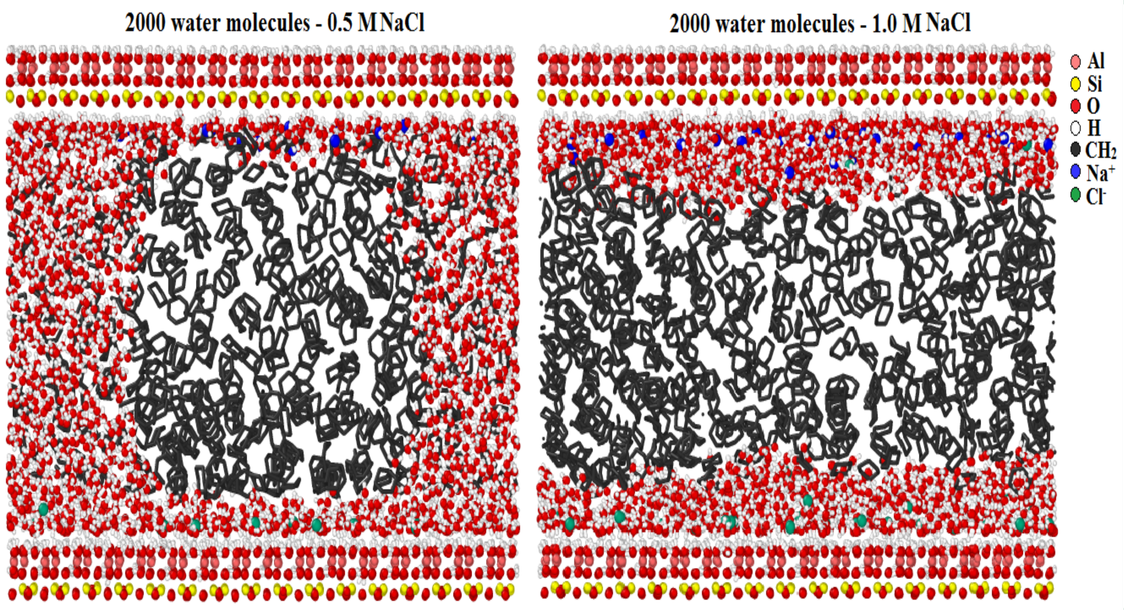
Cyclohexane-water

- **Octahedral sheet:** strong hydrophilic character due to presence of both acceptor and donor sites. The average total number of hydrogen bonds per water molecule exceeds that of the bulk region due to a big contribution from surface-water H-bonding, making it the most energetically-favorable interaction site within the pore.
- **Tetrahedral sheet:** a favorable adsorption site for cyclohexane due to LJ interactions with the basal oxygens. Due to exposure of only acceptors, water structure is perturbed in the vicinity of this surface, making it the least energetically-favorable region for water. Wettability of this surface is dependent on the pore's water content.
- Increasing the amount of water is not a practical solution for elimination of cyclohexane's interaction with the tetrahedral sheet ➡ Water-surface interactions can be improved by addition of salt.



Cyclohexane-water-salt

- Adsorption of Cl^- and Na^+ ions to the octahedral and tetrahedral sheet
- Structure-making role of the ions manifested by a substantial increase in the number of intermolecular hydrogen bonds near both surfaces
- Formation of a complete water monolayer on the tetrahedral sheet at the concentration of 0.5 M
- Complete phase-separation of water and cyclohexane at the concentration of 1.0 M, due to screening of the surface potentials by the adsorbed counter-ions
- The increase in the water's ionic strength leads to shortening of the surface potentials' decay lengths, thus preventing them to overlap in a wide range of distance away from each surface ➡ Breakage of the water-bridge.



FES PROJECT OVERVIEW

T08 P01

Non-Aqueous Extraction (NAE) of oil from the oilsands could significantly reduce the energy and fresh-water consumption. The ultimate goal in this project is contributing to the development of this method by providing solutions for elimination/minimization of the amount of residual solvent in the extraction gangue.

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