MEL zeolite nanosheet membranes for water purification: insights from molecular dynamics simulations

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Abstract

MEL-type zeolite was selected as a typical porous material to theoretically capture the purification scenario of a model landfill leachate comprising $PbCl_2$ and $CuCl_2$ varying the pressure (2.4–48 MPa). Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) was applied to simulate the equilibrium state (0.5 ns) and dynamics of Pb^{2+}, Cu^{2+} and Cl^- and water molecules (4 ns). Overall, the flux through the MEL membrane was increased by the increase of pressure. Lennard-Jones potential was used to explain non-bonded interactions between the membrane and ions as well as water molecules, in terms of values of energy and snapshots were taken from the evolution of purification phenomenon. The molecular patterns of accumulation of ions in the vicinity of zeolitic membrane were also captured as functions of the energies of the interaction between the contaminants and porous membrane. Mean square displacement (MSD) variation was indicative of the effect of pressure on dynamics of heavy metal separation; higher energies obtained at higher pressures, as reflected in alteration of van der Waals (vdW) force between ions and water molecules. The membrane revealed rejection above 70% for Pb^{2+}, and almost 100% against Cu^{2+} and Cl^-, respectively. Density of water remained almost 1 g cm^3, but depending on population of water molecules decreased after passage into the zeolite membrane.