**Molecular dynamics simulations of the adsorption of partially hydrolyzed polyacrylamide on kaolinite edge surfaces in saltwater for a range of pH values: Effect of temperature**

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The adsorption of partially hydrolyzed polyacrylamide (HPAM) polymer chains on kaolinite particles is key in solid-liquid separation processes that seek to recover water in mineral processing. In this work, computational molecular dynamics is used to study the water-kaolinite interface in the presence of HPAM under conditions of high salt concentration and wide pH range. The salts used are some of the most common in seawater. Water clarification processes occur at very different temperatures at different times of the year, however the effect of temperature has practically not been studied. First, quantum mechanical calculations are used to describe the negative charging on the edge surfaces of the kaolinite at and above its point of zero charge. Then, molecular simulations are used to evaluate the effect of temperature on the adsorption of ions and HPAM chains on the edges of kaolinite particles. The saltwater contains different salts, where the anion is chloride and the cation an alkali metal or alkaline-earth metal, in all cases concentration is as high as 0.6 M. It is also considered a brine that imitates seawater, with an ionic strength of 0.6 M and the simultaneous presence of Cl-, Na+, SO42-, Mg2+, Ca2+ and K+. The pH range of the simulations is 7 to 11 and the temperature range is 273 to 313 K. The results show that the ions compete for the edge surfaces of the kaolinite, although water-structure maker ions always adsorb better than water-structure breaker ions. An interesting result is that the adsorption of HPAM is promoted by the salts with maker cations and is hindered by the salts with breaker cations. Temperature has a significant impact. We hope these results can contribute to the decision making in water clarification processes in mineral treatment.

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