
Potential of Mean Force between Silica Particles in Aqueous Solutions from Molecular Simulations: Effect of Interparticle Distance and Salinity

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Abstract

1 Introduction

Colloidal interactions within saturated porous media have attracted increasing attention in recent decades due to the remarkable ability of colloids to capture and transfer non-aqueous phases. This capability allows them to control the physico-chemical characteristics of the solution and affect the poromechanical properties of the media. Understanding and predicting colloidal behaviour within geological formations requires first studying inter-particle couplings at the nanometer level. The underlying mechanisms of colloidal interactions have been well described using the Derjaguin-Landau-Vervey-Overbeek (DLVO) theory, accounting for Van der Waals forces and osmotic repulsion across a broad range of spatio-temporal scales (1,2). Nevertheless, this approach has proven to be inadequate at inter-particle separations below 3 nm, since phenomena such as *electrostatic* attraction in electrical double layers, contact and hydration repulsion dominate hydrodynamic interactions (3). While the nature of colloidal couplings at such ultra-small scales plays a key role in geological processes, such as enhanced oil recovery and groundwater remediation, it remains poorly investigated.

2 Results and Discussion

In this work, an umbrella sampling molecular dynamics technique has been applied to characterize the free energy landscapes of a pair of spherical silica nanoparticles in various aqueous solutions as a function of inter-particle distance. First of all, it has been shown that the ultra-thin fluid layer affects the fluctuations of the interparticle potential of mean force. Particular attention is paid to couplings at distances less than 3 nm. It has been illustrated that non-DLVO forces become important at small inter-particle separations. The limitations of the conventional theory in describing colloidal interactions have been confirmed at close proximity of colloids for different salinity conditions. The present study of the interplays among aqueous silica nanoparticles at the atomistic level needs further investigations to advance the understanding of colloidal phenomena within porous structures.

References

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