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Molecular dynamics simulation of ionic diffusion and mixing phenomena in polymer-enhanced low-salinity waterflooding

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Various studies have confirmed that water salinity and composition significantly impact the efficiency of the waterflooding process. Field-scale operation of low-salinity water injection has been proven to be a cost-effective enhanced oil recovery (EOR) method as well as compatible with environmental regulations. The success of this technique relies on the contact of low-salinity water with the rock surface to alter the wettability of the rock to more water-wetting conditions. However, the salinity of the injected water increases, as it contacts the resident high-salinity reservoir brine which then significantly impairs the efficiency of this technique. Under flowing conditions, two main mechanisms affect the mixing phenomena: hydrodynamic dispersion and molecular diffusion. Our preceding laboratory research has clearly shown that if a small amount of polymer, such as HPAM (partially Hydrolyzed Polyacrylamide) is added to the injection low-salinity water it can significantly reduce the mixing zone by suppressing the diffusion and dispersion phenomena and increase the integrity of the fluid-fluid front. To gain a more in-depth understanding of this process, molecular dynamics simulations were performed to investigate the system at an atomic scale. Polymer molecules were introduced into the low-salinity water and the high-salinity and low-salinity waters were made laterally in contact, under no-flow conditions, to start mixing. Sensitivity analysis was performed on the main factors affecting this phenomenon such as the presence of polymer molecules, the effect of polymer concentration, the salinity of low salinity water, and the salinity of resident brine (i.e., the salinity difference). The results indicate that the time for full mixing is controlled primarily by the effective diffusion coefficient. By adding polymer, the polymer strands and their chemical interaction with the brine ions would act as a diffusion barrier and reduce the diffusivity of low-salinity water, enhance the viscosity, and delay the ionic diffusion phenomenon; thereby reducing the growth rate of the mixing zone. In all cases the mixing zone grew linearly with the square root of time; indicative of Fickian diffusive mixing. Once the diffusivity is reduced, the salinity profile becomes sharper, leading to a more effective low-salinity water effect, and less volume of injecting EOR agent is required at large scales.

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