

عنوان مقاله:

Distribution of Oil, Water, and Ions Near the Neutral Calcite Surface in the Presence of Low and High Salinity Water:
Molecular Dynamics Simulation

محل انتشار:

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خلاصه مقاله:

Low salinity water flooding has a significant impact on the recovery of carbonate reservoirs. In this paper, the molecular dynamics simulation was carried out to investigate the distribution of ions (Na^+ , Cl^- , Ca^{2+} , Mg^{2+} , and SO_4^{2-}), water, and oil molecules near the calcite surface (the temperature of 360 K). The results show that the polar component of oil, compared to the non-polar components, tends more to the calcite surface. Additionally, the bulk of oil in brine-containing environments gradually moves away from the surface. Water molecules exhibit simultaneous movement towards the surface, forming two distinct layers near the surface and hydrating the calcite surface. Based on the water's radial distribution function, it can be observed that the hydrogen atom is closest to the surface within the second layer of water molecules. In contrast, the oxygen atom is in closest proximity to it in the first. Ions displayed concurrent movement towards the surface in conjunction with the motion of water molecules. The ion dispersion gives rise to the forming of an electrical double layer near the surface. Compared to other ions, the closeness of sodium and chlorine ions to the surface leads to creating a layer with a positive charge. The presence of an electrical layer induces the migration of polar oil molecules from the surface. The distribution of Mg^{2+} and Ca^{2+} ions indicates that Mg^{2+} has a stronger surface accumulation tendency than Ca^{2+} .

کلمات کلیدی:

Carbonate Reservoir, Low Salinity Water, Ions, Molecular Dynamics Microscopic Displacement in the Reservoir.
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