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## Contact Angle Measurement and Molecular Dynamics Simulation of Wettability Alteration on Calcite Surface

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This study describes wettability alteration mechanism of calcite surface by low salinity water (diluted seawater) and ion tuned water (regarding to potential determining ions, PDI). The contact angles of brine droplets on calcite surfaces that immersed in oil were measured. The relative ability in modifying the surface wettability of these three ion species (Ca2+, Mg2+ and SO42- ions) thus is evaluated. Contact angles results suggested that 10 times diluted seawater is sufficient to alter the calcite surface into more water-wet. In addition, increasing SO42- and Mg2+ concentration whilst decreasing Ca2+ concentration modify the calcite into more water-wet. Therefore, an ion tuned water which is obtained by manipulating seawater to contain four times SO42- concentration, two times Mg2+ concentration and one-half Ca2+ concentration gives rise to a maximum magnitude of water wetness of calcite surface. Moreover, molecular dynamics (MD) simulation of contact angles has been carried out in order to gain more fundamental understanding on the relationship between wettability and salinity or PDI effect. MD simulation results suggested that SO42- and Mg2+ ions tend to incorporate into calcite lattice and disturb the orientation of water molecules at interface. In general, MD showed a good consistent with experimental results. Therefore, this paper is expected to provide some new insights into low salinity water flooding and ion tuned water flooding in carbonate reservoirs.

## References

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