Contribution ID: **195** Type: **Poster (+) Presentation**

Extension of SAFT equation of state to include calcite wall effect in water properties within water-calcite interface using molecular dynamic simulations

Tuesday, 1 June 2021 20:00 (1 hour)

On the fluid-rock interface, the order of the molecular structure and dynamical properties of fluid deviates from that of the bulk phase and the fluid exhibits a different thermodynamic behavior. To develop an understanding of the fluid-rock interface molecular dynamic (MD) simulation is conducted for water-calcite system. In this study, the results of MD simulations explicitly exhibit the layering transition of water on water-calcite interface. To predict the water properties near calcite wall, we have defined a contribution for Helmholtz energy extended from SAFT equation of state (EOS).In this approach, the confined water molecules interact with calcite surface through a square well energy (ε) estimated by MD simulation at a certain temperature (T). The outcomes of MD simulations confirm the fluctuation of energy, within the confinement, corresponds to the the calcite electrostatic field on the bulk water. The modified SAFT shows a good agreement with MD observations and the introduced model can predict the thermodynamic properties of water at systems with low water content.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

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