Contribution ID: **40** Type: **Oral Presentation**

Extension of the SAFT equation of state to capture the effect of the solid wall into the confined fluid properties: using molecular dynamic simulation

Tuesday, 31 May 2022 17:15 (15 minutes)

The thermodynamic characteristics of water confined inside a nano-mineral pore differs from the bulk properties because of the competition between water-water and wall-water attractions near the solid walls. We used molecular dynamic (MD) simulation, to capture the influence of the solid walls of a slit shape calcite nanopore on the confined water provided in different widths namely 2 nm, 3 nm, 4 nm and 5 nm. The simulations are conducted with NVT ensemble at T = 300 K, 350 K, 400 K, and 450 K while each simulation run is completed within 6 ns. The results shows the density and total energy near the pore wall increases with temperature. To determine the new properties imposed by the nano-calcite pore, an equation of state (EoS) was developed based on the statistical association fluid theory (SAFT) by introducing a new term for Helmholtz free energy. Within a reliable absolute relative error (ARE), the results of the modified SAFT overlap with the outcomes of MD simulation. This approach can be applied in predicting the fluid properties near wall, which is the concern of several fields such as CO2 storage, hydrogen storage and enhanced oil recovery (EOR) and etc.

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Participation

Online

Primary authors: Mr AHMADIGOLTAPEH, Sajjad (University of Oslo); Dr MIRI, Rohaldin (Iran University of Science and Technology (IUST)); Dr AAGAARD, Per (University of Oslo); Dr HELLEVANG, Helge (University of Oslo)

Presenter: Mr AHMADIGOLTAPEH, Sajjad (University of Oslo)

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