MOLECULAR MODELING OF INTERFACIAL TENSION AND CONTACT ANGLES AT RESERVOIR CONDITIONS

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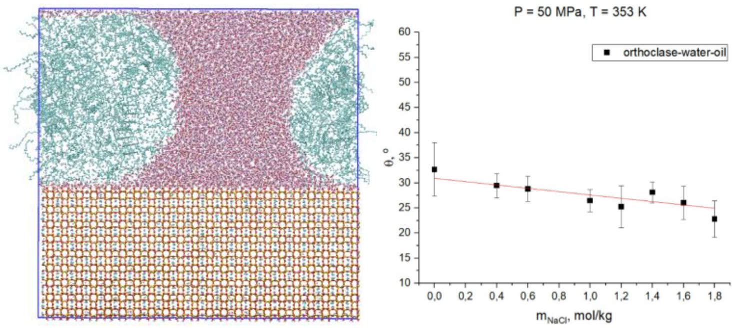
This work presents an experimentally informed molecular simulation study of wettability at feldspar–fluid–fluid interfaces under reservoir conditions. Contact angles at the three-phase contact line are evaluated as a function of temperature, pressure and brine salinity for feldspar–oil–brine, feldspar–oil–methane, and feldspar–brine–methane contact lines. Both K^+ and Na^+ feldspar (orthoclase and albite) are considered. Solid–fluid interaction parameters are quantitatively validated against available ambient-condition contact-angle measurements for water–decane–feldspar systems, and the validated models are transferred to reservoir conditions.

Crude oil is represented as a real-component mixture of alkanes and arenes based on chromatographic and distillation experimental data, with special attention to methane present at reservoir conditions [1]. Contact angles are computed using a robust, adjustable protocol [2].

The resulting dataset enables sensitivity analysis of feldspar wettability to reservoir conditions and composition. The simulation results are parameterized with multivariate linear regression, providing a compact predictive correlation for contact angle as a function of temperature, pressure, gas content, and brine salinity for feldspar-containing rock formations.



(left) Snapshots of molecular configurations at orthoclase – oil – water contact line
(right) dependence of the contact angle on brine salinity at fixed *T* and *p*

1. Khovental P., Kopanichuk I., Kevorkyants R., Maerle K., Yurchenko A., Vishnyakov A. Reservoir oil interface with brine studied with real-component molecular model // Journal of Molecular Liquids. 2025. Vol. 424. Art. 127019.

2. Semenchuk A.A., Kondratyuk N.D., Kopanichuk I.V. PANDA: Predicting angle from nanoscale density analysis // Coll. Surf. A. 2025. Vol. 708. Art. 135994.