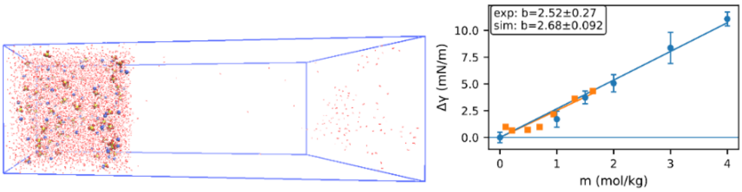
MOLECULAR SIMULATION AND THERMOMECHANICAL PREDICTION OF BRINE-VAPOR TENSION AT RESERVOIR CONDITIONS

Ryazanov S.V.(1,2)*, Vishnyakov A.*(1,2)*, Kalikin N.N.*(3,4)*, Alshammari S.*(5)
(1) Moscow State University
119991, Moscow, Leninskie Gory, 1
(2) Aramco Innovations
117105, Moscow, Varshavskoe Highway, 9, bld. 1
(3) HSE University
123458, Moscow, Tallinskaya st., 34
(4) G.A. Krestov Institute of Solution Chemistry
153045, Ivanovo, Akademicheskaya st., 1
(5) Saudi Aramco EXPEC Advanced Research Center
34466, Dhahran, Saudi Arabia, Gharb Al Dhahran, 8352, 3913

Accurate prediction of interfacial tension (IFT) between reservoir fluids across broad ranges of temperature, pressure, salinity, and gas composition is essential for planning upstream processes, in particular for CO_2 mineralization. However, reservoir-condition IFT data is scarce and often inconsistent, especially for concentrated multicomponent brines (Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, SO_4^{2-}, HCO_3^-) and vapors (CH_4, CO_2, H_2S). High-pressure measurements for H_2S-rich vapors are very laborious and expensive due to safety concerns. This work reports experimentally informed molecular simulation studies of brine—vapor interface at ambient and reservoir conditions. The effects of brine and vapor composition, pressure and temperature are systematically examined. Good agreement with experiments is achieved for most of the system of interest, and systematic correction are proposed for sulfates and carbonates. Experimental data and simulations are applied in parameterization of a thermomechanical model [1], in which surface tension is obtained from the mismatch of normal and tangential stresses derived from the grand thermodynamic potential of an inhomogeneous Coulomb fluid. The theory is fitted to diverse systems using a minimal number of physically interpretable parameters related to the structural characteristics of the interfacial layer obtained in molecular modeling. The final outcome is a compact predictive model (with uncertainty bounds reflecting experimental scatter) suitable for reservoir-scale workflow integration.



(a) Snapshot of the aqueous $MgSO_4$ solution–air interface at *m* = 0.64 mol kg^{-1},
(b) dependence of the interfacial tension on brine salinity for $MgCl_2$

1. Budkov Y.A., Kalikin N.N., Brandyshev P.E. Surface tension of aqueous electrolyte solutions. A thermomechanical approach // J. Chem. Phys. 2024. V. 160. № 164701.