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Unraveling fluid-fluid interfaces through molecular simulations and machine learning

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A current challenge in the O&G industry is the control of fluid-fluid and fluid-solid interfacial properties to promote increased production from mature wells and unconventional sources. Recently, the injection of low salinity brine stand out among the techniques of enhanced oil recovery (EOR), both for its economic and environmental appeal. We investigate the relationship between the structural properties of fluids and the interfacial tension of the oil/brine system by coupling molecular dynamics (MD) simulations and data analysis using machine learning (ML) to extract trends and correlations. The analysis was based on the previous MD trajectories involving brine-oil interfaces [1]. The fluids include brines with varying mono and divalent ions and salinity concentration interfaced with mono to complex multicomponent oil systems. The detailed characterization of the interfaces includes structural, thermodynamics and transport properties to analyze interface order parameters, such as entropy, kurtosis of the orientation angles of molecules at the interface and in the bulk phase. Using the xg boost technique, we identify and ranked the structural features that most influence interfacial tension. The density of aromatics and paraffinic appeared in the classification list among the relevant properties. The interfaces have an anisotropy, and the aromatic rings present a high ordering at the interface with a preferential orientation parallel to the plane. The interplay between interfacial tension and the width of the oil-brine interface could be represented by a linear model. Finally, we developed regression models with very reasonable interfacial tension predictions, indicating that the ML models built were able to capture the information embodied on the fluid-fluid interfaces at a molecular level. The combination of MD and ML can describe the oil/brine interfaces innovatively, allowing to know details not revealed by experimental techniques.

[1] Kirch et al., *ACS Appl. Mater. Interfaces* 2020, 12, 15837