# Gulf of Mexico Produced Water: Characterization and Simulation

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Produced water remediation to NPDES target levels can represent a significant cost for oil production in the Gulf of Mexico. Off-shore analysis and remediation of produced water is expensive, and the relatively high polar content of Gulf of Mexico crude oil also means a higher solubility of organic components in the aqueous phase. In addition, neither are the identities of the water-soluble components well known, nor are their concentrations in the produced water brines. These concentrations will be affected by physical variables such as pH and temperature, but also by the depth of the formation and the age of the well. This work endeavors to address part of this gap in the knowledge base, both through characterization of produced water simulants associated with actual crude oil samples from the Gulf of Mexico, and by modeling of the produced water/crude system using chemical thermodynamics. Because of the focus on semi-volatile components, the chemical system was modeled as a liquid-liquid equilibrium with activity coefficients based on a UNIFAC functional group analysis. A Monte Carlo sampling method was introduced to allow uncertainties in the input data to be reflected in the results of the computation. The model has successfully reproduced parametric studies carried out at ORNL, allowing explanation of changes in solubility observed with variations in pH and temperature.