Modeling of Water-Soluble Organic Content in Produced Water

FEW FEAC329

Program

This project was funded through DOE's Natural Gas and Oil Technology Partnership Program. The program establishes alliances that combine the resources and experience of the nation's petroleum industry with the capabilities of the national laboratories to expedite research, development, and demonstration of advanced technologies for improved natural gas and oil recovery.

Project Goal

The objective of this project is to develop a model that will allow the prediction of the production of water-soluble organics as a function of measurable parameters, such as crude composition, formation characteristics, and produced-water composition.

Performers

Oak Ridge National Laboratory (ORNL)
Oak Ridge, TN

Project Results

The project has provided a computational tool based on analysis and modeling of oil/brine samples, to be used to predict the water-soluble organic content in brines associated with deep-well oil production. ORNL has summarized and published results of the Petroleum Environmental Research Foundation collaboration that led to the study of water solubles in produced water.

Benefits

The computational model could be used prior to production from new facilities to assist in the development of a more selective and focused approach to produced water cleanup, leading to cost savings and reduced environmental impact.

Background

Large amounts of brine are often associated with oil and gas production. Because these produced waters are in contact with oil at high pressures, they can become contaminated with water-soluble organic compounds. The discharge of produced water in the Gulf of Mexico is regulated by NPDES (National Pollutant Discharge Elimination System) permits, which specify that total oil and grease in the water be below a daily maximum of 42 ppm. Analysis of the produced water for total petroleum hydrocarbons by Environmental Protection Agency methods 413.1 or 1664, however, does not distinguish between carboxylic acids/other polar compounds and more environmentally harmful hydrocarbons. Hence, remediation of a billion barrels of produced water per annum in the United States is based on aqueous organic concentrations that exceed the actual content of oil and grease. The goal of the project is to provide a computational tool, based on analysis and modeling of oil/brine samples, to predict the water-soluble organic content in brines associated with deep-well oil production. Such a model could be used prior to production from new facilities to assist in the development of a more selective and focused approach to produced water clean-up, lending to cost savings and reduced environmental impact.

Project Summary

The type and amount of organics that are soluble in produced water is not well understood, leading to inefficiencies in produced water clean-up prior to its discharge into the ocean. Industry participants and ORNL embarked on a study of organic solubility in produced water, including characterization of the organic component in produced water and modeling of its solubility. The characterization of the produced water is complete and shows that the water-soluble component is primarily polar with a discernible trend in increased solubility with increasing pH.

To model aqueous-hydrocarbon systems, ORNL successfully used a simple liquid-liquid equilibrium model to fit the pH-dependence data that were generated in a crude-oil/simulated brine system. The model incorporates the acidity of the polar components. Results of calculations agree with the trend seen in the experimental results, where methylene-chloride extractable range material (particularly C_{10}-C_{20}) becomes more soluble as the pH increases beyond 7. This is because of increased deprotonation in the basic aqueous phase.

The advantage of a thermodynamic equilibrium model is that changing conditions, such as temperature dependence and salinity, can be incorporated into the expressions for the activity coefficients. Volatile components and the dependence of solubility on pressure can be introduced with an additional gaseous phase, represented by an equation of state.

Current Status (October 2005)

The project is in its final year.