Modeling of Water-Soluble Organic Content in Produced Water

ORNL, Chevron, Phillips, Shell, and Statoil

Joanna McFarlane

NGOTP Upstream Environmental Technology Review

Houston, October 24, 2001

Water-Soluble Organics Are Increasingly an Industry-Wide Problem

- Meeting regulatory discharge limits for dissolved organics is a challenge
- Early data for the Gulf of Mexico wells indicate that dissolved organics will increase from deep-water wells
- The chemistry involved in production of water-soluble organics is not understood
  - Cannot predict generation for new wells
  - Cannot predict treatment requirements

Four Oil Companies and ORNL Collaborate Water-Solubles Project (PERF 98-04)

- **Characterize water-soluble organics in produced water**
- ***Develop a model to predict production of water-soluble organics***
- **Develop treatment methods for water-soluble organics**

ORNL Proposal Develops Model To Complete PERF 98-04 Scope

- **Objective: Model water-soluble organics in produced water as a function of experimental variables**

- **Ultimate goal: Provide model to predict water-soluble organic content in produced water from deep-well sites based on field variables**

Technical Approach

- Stage 1
  - Empirical analysis of PERF 89-04 data on water-soluble organic content in simulated produced water
- Stage 2
  - Extend model to calculate amounts of organic compounds present in produced water from other oil fields
- Stage 3
  - Revise model to allow predictions based on field or production variables as well as experimentally measured variables

PERF 98-04 Characterization Data Show Chemical Effects on Solubility

- pH
- Compound hydration
- Salinity
- Effects of mixing
- Water cut

PERF 98-04 Characterization Data Show Physical Effects on Solubility

- Temperature
- Pressure
- Surface-to-volume ratio, absolute volume
- Turbulence, rapid changes in physical conditions
- Suspended solids, dissolved organic materials, surfactants

1. Empirical Analysis of PERF 98-04 Data

- Focus on the aqueous solubility of *groups* of semi volatile compounds that are derived from crude oil

- Use empirical model to quantify how the following factors influence hydrocarbon solubility in produced water:
  - pH
  - Salinity
  - Pressure
  - Temperature

2. Application of Model to Crude-Brine Data

- Acquire additional produced water characterization data sets from other oil fields
  - Gulf of Mexico
  - North Sea
- Compare model calculations with these data sets
- Recommend changes to model or additional experimental analyses to fill gaps in data sets
- Extend model by including the following:
  - More experimental variables
  - Physical models (chemical thermodynamics)

3. *Refinement of Model for Use with Field Variables*

- Select relevant variables
  - Lab based
  - Field based

- Use statistical model to predict water-soluble organic content of produced water
  - Identify the most important variables correlated with solubility
  - Test model against data from existing oil fields
  - Predict organic content in produced water from new oil fields

Industry Participation

- Project planning and oversight
  - Provide guidance in model development
  - Make recommendations for additional characterization tests if required
  - Facilitate liaison with other PERF projects (e.g., UMIST) and with contractors
- Produced water-crude data sets
  - Industrial measurements in laboratory and offshore
  - Crude-brine samples for further characterization at ORNL
- Advice on relevant field parameters for predictive model
- Testing and evaluation of model with feedback to developers

Project Schedule

- First year
  - Evaluate trends in PERF 98-04 characterization data
  - Develop empirical model to describe trends
  - Select additional data sets for comparison with model calculations
- Second year
  - Evaluate empirical model by comparing results with additional data sets
  - Refine empirical coefficients to reflect accurately a larger data set
- Third year
  - Modify model to use field variables to calculate the solubility of organic components in produced water
  - Document recommended model and parameters for use in model predictions

Project Budget ($ x 10^3)

	FY 2002	FY 2003	FY 2004
ORNL	250	250	250
University	0	0	0
DOE total	250	250	250
Industry (in kind)	150	150	150

Project Impacts

- A model will be developed to predict the *amounts* and *types* of environmentally important classes of organic compounds in produced water, taking into consideration key characteristics of the oil field

- Industrial partners can use this information to accomplish the following:
  - Reduce production of the water-soluble contaminants on existing platforms
  - Develop methods of treatment that are efficient and cost-effective for new oil fields