Test Design Using Numerical Simulations

Center for Petroleum and Geosystems Engineering
The University of Texas at Austin

CPGE

SEAR Workshop
Objectives

- Establish the operating parameters
- Demonstrate to the regulators that hydraulic capture can be accomplished
- Predict the effluent contaminant and surfactant concentration for surface treatment
- Improve understanding of process mechanisms and feedback to laboratory experiments
- Consider optimization, risk reduction, and scaleup
- Assess performance of field data
Role of Numerical Models

• Provide a tool for understanding how variation in subsurface properties can impact SEAR design
• Aid in a more robust design to withstand the uncertainties in site characterization
• Explore alternative strategies and approaches
Benefits

- Understanding of aquifer characteristics under dynamic conditions
- Optimization of surfactant remediation design
- Assessment of problems and risks
- Guide to laboratory program
- Guide to field operations
- Aid in communication with regulators
- Guide to future research
Design Approach

• Establish simulation grid
• Develop Geosystem model based upon characterization data
• Input surfactant and DNAPL properties
• Conduct sensitivity study
• Select optimum design parameters
Numerical Models

• Rathfelder et al., (SURF2D)
  – 2-D, 2-Phase flow solubilization process
• Adeel et al., 1995
  – 2-D, 2-Phase flow, allow for rate limited dissolution
• Ji and Brusseau
  – 1-D, 2-phase flow for solubilization process
UTCHEM Flow and Transport Model: Overview

- 3-Dimensional, variable-temperature chemical compositional simulator
- Third-order finite difference with a flux limiter
- Four phases: water, NAPL, microemulsion, and air
- Vertical and horizontal wells
- Cartesian, radial, and curvilinear grid options
SEAR Field Tests Designed Using UTCHEM

- OU2, Hill AFB surfactant demonstration (AFCEE)
- OU2, Hill AFB surfactant/foam demonstration (AATDF)
- Naval Station Pearl Harbor
- MCB Camp Lejeune
- OK TOOLS
- OU2, Hill AFB full-scale
- OU1, Hill AFB
Field Design Variables

- Well pattern and well rates
- Hydraulic control well locations and rates
- Location of well screens
- Location of multilevel samplers and frequency of sampling
- Mass of injected surfactant/cosolvent
- Composition of surfactant solution
- Mobility control (i.e., polymer or foam)
- Surface treatment facilities
Critical SEAR Remediation Variables

- Surfactant phase behavior
- Interfacial tension
- Surfactant adsorption
- Viscosity
- Density
- Mass transfer and diffusion
- Surfactant biodegradation
- Polymer compatibility and properties (if used)
- Cost and availability of chemicals
Areal View of Simulation Grid
MCB Camp Lejeune SEAR Test: 10,000 gridblocks, 25x25x16 mesh

Injection & Hydraulic Control Wells
 Extraction Wells

North Wall of Bldg. 25
Areal View of Simulation Grid
OU2, Hill AFB

7,296 gridblocks
32x19x12 mesh

LEGEND
- Extraction Well
- Injection Well
- Monitoring Well

Boundaries of Channel
Model Input: Geosystem Model Data

- Permeability
- Porosity
- Initial DNAPL volume and saturation distribution
- Clay aquitard elevations and properties
- Contaminant and groundwater fluid properties (density, viscosity, interfacial tension, water composition, and DNAPL solubility)
- Wellfield data
- Natural hydraulic gradient
Upper Surface of Clay Aquitard Beneath Building 25 at MCB Camp Lejeune
Geosystem Cross Section of MCB Camp Lejeune DNAPL Zone

- Ground Surface
- Varsol Smear Zone
- DNAPL Zone

- Castle Hayne Aquifer
- EX01 ML-1 IN01 ML-4 EX04
- 15 ft
- 0 5 10 15 20 34
- Depth (ft bgs)
- DNAPL
- Clay Aquitard
- Clayey Silt
- Fine Sand and Silt

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Permeability Distribution
Hill AFB SEAR Test

IN = injection well
EX = extraction well
HC = hydraulic control well

Permeability, Darcy

2  5.6  9.2  12.8  16.4  20
Model Input: Process Data

- Phase behavior of surfactant/cosolvent/electrolyte
- Microemulsion properties (density, viscosity)
- DNAPL/microemulsion interfacial tension
- Mass transfer rate
- Relative permeability-capillary pressure-saturation
- Ion exchange
- Adsorption
- Dispersion
Surfactant Phase Behavior vs. Electrolyte Concentration

Type I  Type III  Type II

Electrolyte (Salt) Concentration

Water Phase
Microemulsion Phase
NAPL Phase
Volume Fraction Diagram for Alfoterra© 145 (PO)₄ SO₄Na with DNAPL at 25ºC

- DNAPL
- Microemulsion Phase
- Aqueous Phase

4 wt.% surfactant
16 wt.% IPA
pH of site tape water: 8.59

Volume Fraction

Concentration of CaCl₂, wt.%

0.0 0.2 0.4 0.6 0.8 1.0

0.10 0.15 0.20 0.25 0.30
Critical Model Output

- Effluent concentrations of contaminant, surfactant, and cosolvent, which are critical to the surface treatment program
- DNAPL saturation reduction within the well field
- Concentrations of contaminant, surfactant, and cosolvent at the monitoring locations
- Water level fluctuations due to the injected chemicals
- Volume of free-phase product recovered
- Mass of contaminant, surfactant, and cosolvent recovered
- Final concentrations of contaminant and all the injected chemicals
Sample Model Input: UTCHEM Simulation of Camp Lejeune Flood

<table>
<thead>
<tr>
<th>Process</th>
<th>Rate (gpm)</th>
<th>Surfactant/IPA (wt %)</th>
<th>CaCl₂ (wt%)</th>
<th>Inj. Time (days)</th>
<th>Cum. Time (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preflush</td>
<td>Injection (L): 0.1334 Injection (U): 0.0800 Extraction: 0.1667 Hydraulic control: 0.2000</td>
<td>0</td>
<td>0.22</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Surfactant flush</td>
<td>Injection (L): 0.1334 Injection (U): 0.08 Extraction: 0.1667 Hydraulic control: 0.2000</td>
<td>4/16</td>
<td>0.22</td>
<td>48</td>
<td>54</td>
</tr>
<tr>
<td>Water</td>
<td>Injection (L): 0.20 Injection (U): 0.08 Extraction: 0.25 Hydraulic control: 0.30</td>
<td>0</td>
<td>0.1</td>
<td>16</td>
<td>70</td>
</tr>
<tr>
<td>Final PITT</td>
<td>Injection (L): 0.20 Injection (U): 0.08 Extraction: 0.25 Hydraulic control: 0.30</td>
<td>0</td>
<td>0.1</td>
<td>42</td>
<td>112</td>
</tr>
</tbody>
</table>

L = lower screen; U = upper screen

Test Design Using Numerical Simulations
## Sample Model Output: UTCHEM Simulation of Camp Lejeune flood

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>EX01</td>
<td>35.06</td>
<td>0.0</td>
<td>3,363</td>
<td>982</td>
</tr>
<tr>
<td>EX02</td>
<td>35.08</td>
<td>0.0</td>
<td>6,831</td>
<td>2,013</td>
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<tr>
<td>EX03</td>
<td>5.574</td>
<td>0.0</td>
<td>3,391</td>
<td>995.2</td>
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<td>EX04</td>
<td>35.41</td>
<td>0.07</td>
<td>6,564</td>
<td>1,940</td>
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<tr>
<td>EX05</td>
<td>39.39</td>
<td>0.0</td>
<td>6,703</td>
<td>1,984</td>
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<tr>
<td>EX06</td>
<td>13.66</td>
<td>0.3022</td>
<td>3,635</td>
<td>1,071</td>
</tr>
<tr>
<td>TOTAL</td>
<td>164.174</td>
<td>0.3722</td>
<td>30,487</td>
<td>8,985.2</td>
</tr>
</tbody>
</table>
Model DNAPL Saturation Predictions
17.5 ft bgs at MCB Camp Lejeune Site

Initial:

Final:
Dissolved PCE Concentration at Well EX01
MCB Camp Lejeune SEAR Test

![Graph showing dissolved PCE concentration over time](image)

- **Field Data**
- UTCHEM (low permeability)
- UTCHEM (high permeability)
Dissolved PCE Concentration at Well EX01
MCB Camp Lejeune SEAR Test

UTCHEM Model

Field Data

Test Design Using Numerical Simulations
Surfactant Concentration at Well EX01
MCB Camp Lejeune SEAR Test

- UTCHEM Model
- Field Data

Effluent IPA and Surfactant Concentration, wt. %

Time Since Surfactant Injection, days

IPA

Surfactant
Contaminant Concentration at Well SB-1
Hill AFB SEAR Test

Concentration, mg/L

UTCHEM Prediction

GC Contaminant Field Data

Surfactant injection begins
8/7/96
Surfactant injection ends
8/31/96
Surfactant Concentration at Well SB-1
Hill AFB SEAR Test

Field Data
UTCHEM Prediction
Conclusions

• Modeling is beneficial and feasible for SEAR design
• Predictive modeling should be included in work plans submitted before SEAR
• Modeling can be used to interpret field data after SEAR
• Modeling can be useful for all DNAPL remediation processes
Any Questions?

SEAR