NUMERICAL MODELING OF PARTIAL SATURATION IN SANDS INDUCED THROUGH TRANSPORT AND REACTIVITY

SUTRA-BUBBLE

Professor M. K. Yegian
Seda Gokyer, Ph.D. Candidate

NEESR Project: Induced Partial Saturation (IPS) Through Transport and Reactivity for Liquefaction Mitigation

(Grant Number: CMMI-1134940)
**SUTRA – BUBBLE**

- COMPUTER PROGRAM TO MODEL PARTIAL SATURATION IN SANDS INDUCED THROUGH TRANSPORT AND REACTIVITY

**Governing Equation**

\[
\{S_u \rho S_{wp} + \varepsilon \rho S_{bb} \left[ \frac{(1-S_u^b)}{P_b} \right] \frac{\partial P}{\partial t} + \varepsilon S_u \frac{\partial P}{\partial t} \frac{\partial C}{\partial t} - RT \varepsilon \rho S_{bb} \left( \frac{S_u^b}{P_b} \right)^2 \frac{\partial P}{\partial t} \partial_{\text{ideal gas law}} \right\}
\]

\[
\text{S} - \varepsilon \text{V} \left[ \frac{k_k}{\mu} \right] = Q_p
\]

**Injection of sodium percarbonate solution**

- Inj. Pres. = ?
- Inj. Conc. = ?
- Inj. Duration = ?

**Sand**

- S = 100%
- S < 100%

**Concentration of solute**

- time

**Moles of gas bubbles**

- time

**Degree of saturation**

- time

**Fluid mass balance**

**Ideal gas law**

**Darcy’s law**

**S = f (x,y,z,t)**

**Injection nodes**

**Computer simulation**
CONSTITUTIVE MODELS IN SUTRA-BUBBLE – CONT’D

LABORATORY EXPERIMENTS FOR CONSITUTIVE MODELS

Relative permeability of soil

\[ k_r = \frac{k_{PS}}{k_{FS}} \]

- permeability for partially saturated specimen

\[ k_{FS} \] - permeability for fully saturated specimen

\[ k_r = S^\delta \]

Rate of reaction for gas generation

\[ C(t) = (C_0) \exp(-rt) \]

\[ \nu_b(t) = 1 - (\nu_{b0}) \exp(-rt) \]
Relative permeability of soil

\[ k_r = \frac{k_{PS}}{k_{FS}} = S^\delta \]

- used in SUTRA-Bubble model

\[ k_{PS} \] - permeability for partially saturated specimen

\[ k_{FS} \] - permeability for fully saturated specimen

<table>
<thead>
<tr>
<th>Specimen 1 - Fully Saturated (FS)</th>
<th>1.00</th>
<th>0.83</th>
<th>0.056</th>
<th>0.71</th>
<th>1.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen 2 - Partially Saturated (PS)</td>
<td>1.00</td>
<td>0.40</td>
<td>0.050</td>
<td>0.71</td>
<td>1.00</td>
</tr>
<tr>
<td>Specimen 3 - Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.43</td>
<td>0.049</td>
<td>0.77</td>
<td>0.79</td>
</tr>
<tr>
<td>Specimen 4 - Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.23</td>
<td>0.048</td>
<td>0.77</td>
<td>0.76</td>
</tr>
<tr>
<td>Specimen 3 - Partially Saturated (PS)</td>
<td>0.66</td>
<td>0.22</td>
<td>0.024</td>
<td>0.80</td>
<td>0.40</td>
</tr>
<tr>
<td>Specimen 4 - Partially Saturated (PS)</td>
<td>0.66</td>
<td>0.22</td>
<td>0.027</td>
<td>0.80</td>
<td>0.40</td>
</tr>
<tr>
<td>Specimen 3 - Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.90</td>
<td>0.020</td>
<td>0.75</td>
<td>0.35</td>
</tr>
<tr>
<td>Specimen 4 - Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.66</td>
<td>0.019</td>
<td>0.75</td>
<td>0.33</td>
</tr>
<tr>
<td>Specimen 4 - Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.66</td>
<td>0.023</td>
<td>0.75</td>
<td>0.39</td>
</tr>
</tbody>
</table>
CONSTITUTIVE MODELS IN SUTRA-BUBBLE - CONT’D

LABORATORY EXPERIMENTS FOR CONSTITUTIVE MODELS

Rate of gas generation

**Generation of Oxygen Bubbles in Sand**

- $C_{eqv} = 0.76\%$
- $r_{0.76\%} = 0.000133 \text{ (1/sec)}$

- $C_{eqv} = 0.38\%$
- $r_{0.5\%} = 0.0000833 \text{ (1/sec)}$

Fitted gas bubble generation relation in SUTRA-Bubble

\[
r = 0.000133 \text{ (1/sec)} - C_{eqv} = 0.76\%
\]

\[
r = 0.000083 (1/sec) - C_{eqv} = 0.38\%
\]
VALIDATION OF SUTRA-BUBBLE WITH LABORATORY EXPERIMENTS

LARGE SAND SPECIMEN IN A GLASS TANK
EXPERIMENTS FOR VALIDATION OF SUTRA-BUBBLE

Test 1 and Test 2

Measurements made to validate SUTRA-Bubble:

- Inflow/Outflow rates and pore water pressures
- Rate of transport of chemical solution during injection – using Electrical Conductivity Probes
- Degree of saturation in soil – using Electrical Conductivity Probes
**EXPERIMENTAL TEST SET UP**

Picture shows the experimental set up with measurement instruments including electrical conductivity meters and data acquisition system.
EXPERIMENTAL TEST SET UP - CONT’D

- Pore pressure transducers – PPT
- Electrical Conductivity – EC Probe
- Injection Tube
- Kulite XCL– 11-250
- Druck PDCR 81
- Meters to read the EC probes
- Two electrodes measuring electrical resistance
### Final locations of instruments for both Test 1 and Test 2

![Injection tip image]

- **PPT** - Pore pressure transducer
- **EC** - Electrical Conductivity Probe
- Each square side is 5 cm

### Table of parameters of injection

<table>
<thead>
<tr>
<th>Test</th>
<th>e</th>
<th>Depth of inj. tube</th>
<th>Inj. pressure − ΔH (TIP)</th>
<th>Inj. duration</th>
<th>Inj. concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Test 1</strong></td>
<td>0.70</td>
<td>Water inj. 25.5 cm</td>
<td>26 cm</td>
<td>5 min</td>
<td>0%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IPS inj. 25.5 cm</td>
<td>26 cm</td>
<td>13 min</td>
<td>1% (by weight)</td>
</tr>
<tr>
<td><strong>Test 2</strong></td>
<td>0.72</td>
<td>Water inj. 25.5 cm</td>
<td>26 cm</td>
<td>5 min</td>
<td>0%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IPS inj. 25.5 cm</td>
<td>26 cm</td>
<td>13 min</td>
<td>0.5% (by weight)</td>
</tr>
</tbody>
</table>
RESULTS AND DISCUSSIONS

Results from TEST 1

Inflow and pressure measurements

Cumulative flow of water

Test 1

Inflow, gr
Outflow, gr

$q_{ave} = 1944 \text{ gr/min}$
$q_{ave} = 1892 \text{ gr/min}$

end of injection 13 min

Injection of water - Test 1

$\Delta H (\text{TIP}) = 26 \text{ cm}$

$\Delta H = 20.5 \text{ cm}$

Hydrostatic pressure

Injection of sodium percarbonate solution

$\Delta H (\text{TIP}) = 26 \text{ cm}$

$\Delta H = 20 \text{ cm}$

Hydrostatic pressure
RESULTS AND DISCUSSIONS

Results from TEST 1

**Outflow measurements**

TEST 1

$S_{AVE}$ in the zone of partial saturation using outflow measurements:

$(\text{Outflow} - \text{Inflow}) \text{ at } 360 \text{ minutes} = (\Delta V_{\text{water}}) = (V_{\text{bubble}}) = 4292 \text{ cm}^3$

$(V_{\text{c}}) = 27310 \text{ cm}^3$ for total specimen

Partial saturated zone = 55% of the total volume

$(V_{\text{c}}) \text{ for partially saturated zone} = 27310 \times 0.55 = 15021 \text{ cm}^3$

$(S_{AVE}) = (V_{\text{c}} - V_{\text{bubble}}) / V_{\text{c}} = (15021 -4292)/15021 = 0.71$
RESULTS AND DISCUSSIONS

Results from TEST 1

Transport of chemical solution – Electrical Conductivity measurements

- Solution arrives at the locations of probes EC1 to EC9.
- Solution transports ~ 25 cm away from injection.
RESULTS AND DISCUSSIONS

Results from TEST 1

Degree of Saturation – Electrical Conductivity measurements

Archie’s law:

\[ \sigma_t = \frac{1}{a} \times \sigma_w \times \varphi^m \times s^n \]

- \( S \) = Degree of Saturation
- \( n \) = Saturation exponent close to 2
- \( \varphi \) = Porosity
- \( a \) = Tortuosity factor
- \( \sigma_w \) = Electrical conductivity of brine
- \( m \) = Cementation exponent

Assumption: From \( P \) to \( R \) only change in the Archie’s Law if due to change in \( S \)
RESULTS AND DISCUSSIONS

Results from TEST 1

Degree of Saturation – Electrical Conductivity measurements

~ 60% - 70% degree of saturation achieved in the zone of partial saturation
RESULTS AND DISCUSSIONS

Results from TEST 2

**Inflow and pressure measurements**

**TEST 2**

**Cumulative flow of water**

- $q_{ave} = 2400$ gr/min
- $q_{ave} = 2420$ gr/min
- End of injection: 13 min

**Injection of water - Test 2**

$\Delta H$ (TIP) = 26 cm

**TEST 2**

**Cumulative flow of sodium percarbonate solution**

**Injection of sodium percarbonate solution**

$\Delta H$ (TIP) = 26 cm
RESULTS AND DISCUSSIONS

Results from TEST 2

Outflow measurements

TEST 2

$S_{AVE}$ in the zone of partial saturation using outflow measurements:

\[(\text{Outflow} - \text{Inflow}) \times 600 \text{ minutes} = (\Delta V_{\text{water}}) = (V_{\text{bubble}}) = 1483 \text{ cm}^3\]

\[(V_v) = 28311 \text{ cm}^3 \text{ for total specimen}\]

\[\text{Partial saturated zone } \text{ } \Box 40\% \text{ of the total volume}\]

\[(V_v) \text{ for partially saturated zone } = 28311 \times 0.40 = 11324 \text{ cm}^3\]

\[(S_{AVE}) = (V_v - V_{\text{bubble}}) / V_v = (11324-1483)/11324 = 0.87\]
RESULTS AND DISCUSSIONS

Results from TEST 2

Transport of chemical solution – Electrical Conductivity measurements

- Solution arrives at the locations of probes EC1 to EC9 except EC8
- Solution transports ~ 20 cm away from injection.
RESULTS AND DISCUSSIONS

Results from TEST 2

Degree of Saturation – Electrical Conductivity measurements

Archie’s law:

$$\sigma t = 1/a \times \sigma w \times \varphi^m \times S^n$$

S = Degree of Saturation
n = Saturation exponent close to 2
$$\varphi$$ = Porosity
a = Tortuosity factor
$$\sigma w$$ = Electrical conductivity of brine
m = Cementation exponent

Assumption: From P to R only change in the Archie’s Law if due to change in S

![Graph showing electric conductivity over time for TEST 2](image)
RESULTS AND DISCUSSIONS

Results from TEST 2

Degree of Saturation – Electrical Conductivity measurements

~ 60% - 75% degree of saturation achieved in the zone of partial saturation
SUTRA-BUBBLE PREDICTIONS FOR GLASS TANK TEST

Mesh for test specimen

Modeling of injection tube

Permeability (m²)

- 1.75e-010
- 1.17e-010
- 5.83e-011
- 1.00e-030

Injection nodes

Sand

91 cm

25.5 cm

Free surface boundary

Source of flow boundary

Injection tube

Injection tube

Permeability (m²)
### Parameters used in SUTRA-Bubble runs

#### TEST 1 and TEST 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>TEST 1</th>
<th>TEST 2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Size of model</strong></td>
<td>91 cm (L) x 13.5 cm (W)</td>
<td>91 cm (L) x 13.5 cm (W)</td>
</tr>
<tr>
<td><strong>Specimen height</strong></td>
<td>55 cm</td>
<td>55 cm</td>
</tr>
<tr>
<td><strong>Depth of Injection tip</strong></td>
<td>25.5 cm</td>
<td>25.5 cm</td>
</tr>
<tr>
<td><strong>Porosity</strong></td>
<td>0.41</td>
<td>0.42</td>
</tr>
<tr>
<td><strong>Mean Average Permeability</strong></td>
<td>1.5 E-10 m$^2$ *</td>
<td>1.75 E-10 m$^2$ *</td>
</tr>
<tr>
<td><strong>Dispersivity (Long. &amp; Trans.)</strong></td>
<td>1E-4 m</td>
<td>1E-4 m</td>
</tr>
<tr>
<td><strong>Diffusion coefficient</strong></td>
<td>1E-9 m/s</td>
<td>1E-9 m/s</td>
</tr>
<tr>
<td><strong>Coefficient of density change</strong></td>
<td>$\frac{\partial \rho}{\partial C}$</td>
<td>4052 (kg/m³)</td>
</tr>
<tr>
<td><strong>Initial pressure</strong></td>
<td>Hydrostatic pressure</td>
<td>Hydrostatic pressure</td>
</tr>
<tr>
<td><strong>Initial concentration</strong></td>
<td>0 (kg/kg)</td>
<td>0 (kg/kg)</td>
</tr>
<tr>
<td><strong>Actual concentration of H$_2$O$_2$ solution</strong></td>
<td>$C_{(H_2O_2)}$$_{actual}$ = 0.002468 (kg/kg)</td>
<td>$C_{(H_2O_2)}$$_{actual}$ = 0.001234 (kg/kg)</td>
</tr>
<tr>
<td><strong>Injection pressure</strong></td>
<td>$\Delta H$ (TIP) = 26 cm</td>
<td>$\Delta H$ (TIP) = 26 cm</td>
</tr>
<tr>
<td><strong>Duration of injection</strong></td>
<td>13 minutes</td>
<td>13 minutes</td>
</tr>
<tr>
<td><strong>Total duration of the model</strong></td>
<td>360 minutes</td>
<td>600 minutes</td>
</tr>
<tr>
<td><strong>Time increment</strong></td>
<td>10 seconds (for 15 minutes)</td>
<td>10 seconds (for 15 minutes)</td>
</tr>
<tr>
<td></td>
<td>60 seconds (15 to 105 minutes)</td>
<td>60 seconds (15 to 105 minutes)</td>
</tr>
<tr>
<td></td>
<td>360 seconds (105 to 360 minutes)</td>
<td>360 seconds (105 to 600 minutes)</td>
</tr>
<tr>
<td><strong>Mesh size</strong></td>
<td>0.5 cm (hexahedral)</td>
<td>0.5 cm (hexahedral)</td>
</tr>
<tr>
<td><strong>Number of nodes</strong></td>
<td>571872</td>
<td>571872</td>
</tr>
<tr>
<td><strong>Number of elements</strong></td>
<td>543510</td>
<td>543510</td>
</tr>
<tr>
<td><strong>Solver for pressure</strong></td>
<td>Iterative – GMRES</td>
<td>Iterative – GMRES</td>
</tr>
<tr>
<td></td>
<td>Tolerance – 1E-13</td>
<td>Tolerance – 1E-13</td>
</tr>
<tr>
<td></td>
<td># of iterations - 1600</td>
<td># of iterations - 1600</td>
</tr>
</tbody>
</table>
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 1

Inflow/Outflow and pressure measurements

Inflow of solution - SUTRA-Bubble Input

TEST 1

Inflow-Exp
Inflow-Model
Outflow-Exp
Outflow-Model

PPT 1 & PPT 2

PPT 3, 4 & 5

Hydrostatic pressure
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 1

Transport of chemical solution
SUTRA-Bubble output of concentration
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

Transport of chemical solution

SUTRA-Bubble output of concentration & electrical conductivity measurements
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 1

Degree of Saturation

SUTRA-Bubble output of degree of saturation

TEST 1 – 360 minutes
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 1

SUTRA-Bubble output of degree of saturation & Experiment (EC measurements)
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 2

Inflow/Outflow and pressure measurements
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 2

Transport of chemical solution
SUTRA-Bubble output of concentration

TEST 2- 15 minutes

$C_{\text{eqv}(\text{H}_2\text{O}_2)}$ (kg/kg)

22 (H O ) kg/kg C ( )
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

Transport of chemical solution

SUTRA-Bubble output of concentration & Electrical conductivity measurements
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 2

Degree of Saturation

SUTRA-Bubble output of degree of saturation
VALIDATION OF SUTRA-BUBBLE PREDICTIONS

TEST 2

Degree of Saturation

SUTRA-Bubble output of degree of saturation & Experiment (EC measurements)
Findings:

Computer program SUTRA-Bubble was developed to model partial saturation induced through transport and reactivity.

Parameters for constitutive models were determined experimentally.

- Relative permeability \( k_r = S^2 \)
- Rate for gas generation \( r = 0.0001333 \) (1/sec) for \( C = 0.76\% \)
  \( r = 0.0000833 \) (1/sec) for \( C = 0.38\% \)

Measurements from two glass tank tests (Test 1 and Test 2) were compared with SUTRA-Bubble outputs of:

- Flow and pore water pressure measurements
- Concentration of solution – Transport of solution
- Degree of saturation

Observations and Conclusions from the comparisons of glass tank experimental and SUTRA-BUBBLE results:

- Outflow matches well - representing average degree of saturation in zone of flow
- Pressure outputs do not match as well as the other parameters – pressures are very sensitive to soil permeability, assumption of uniform permeability may be rigorous
- Transport of solution matches very well – arrival time of the solution matches very well at each electric conductivity probe location
- Degree of saturation matches quite well
  - The shape of the zone of partial saturation achieved matches quite well
  - At each probe location the final degree of saturation matches well
- In general, the match is better for TEST 1 results compared to TEST 2 results.
- The two experimental tests helped validate SUTRA-BUBBLE