NUMERICAL SIMULATION OF PARTIAL SATURATION 
IN SANDS INDUCED BY FLOW AND CHEMICAL 
REACTIVITY 

A Dissertation Presented 

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ABSTRACT

Moderate to large earthquakes often cause ground failure due to soil liquefaction leading to major and sometimes catastrophic damages to the built environment. Liquefaction is the loss of bearing capacity and shearing resistance of fully saturated sand due to pore pressure buildup in an earthquake leading to geotechnical related failures of engineered structures. While measures have been developed to prevent the occurrence of liquefaction, often they are too costly and/or impractical at sites with existing structures. New liquefaction mitigation measures are being investigated by a number of researchers. “Induced Partial Saturation” (IPS) in sands is an innovative, practical, cost-effective and reliable liquefaction mitigation technique that was developed by researchers at Northeastern University. The IPS technique is based on hydraulic injection and transport of a solution of sodium percarbonate within liquefaction-susceptible sand. The reactivity of the solution results in a slow release of oxygen gas thus reducing the degree of water saturation and permeability of sand. The increase in effective compressibility limits buildup of pore water pressure during an earthquake and thus prevents liquefaction. To better understand, design and implement IPS, it will be necessary to develop a theoretical model for the technique. This research develops the theoretical basis of IPS and implements a numerical solution for modeling partial saturation in sand induced by transport and reactivity of a chemical solution within the pores of the sand. The model is based on coupled differential equations describing three-dimensional, transient, hydraulic
flow and non-linear, advective-dispersive transport of the reactive chemical; coupled with algebraic equations describing the kinetics of the chemical, formation of oxygen gas, and associated decrease in saturation. To simulate partial saturation in sands through transport and reactivity, the computer program SUTRA, developed by the US Geological Survey, was adopted and modified. The new model “SUTRA-Bubble” is a modified version that simulates transient partial saturation created by IPS below the water table. SUTRA-Bubble models partial saturation in soil as a function of chemical reactivity of a solution which is transported through the pores of soil. SUTRA-Bubble also accounts for decrease in permeability of soil as degree of saturation in soil decreases.

SUTRA-Bubble was validated by comparing its predictions with experimental test results. Small-and large scale laboratory experiments were conducted which involved injection of sodium percarbonate solution into sand specimen with controlled pressure and concentration. The SUTRA-Bubble predictions of the extent of the zone of partial saturation and the degree of saturation agreed very well with the small- and large-scale experimental test results. Validation of the model led to verification of the theoretical basis developed for IPS and the conclusion that SUTRA-Bubble, effectively simulates IPS in sands. SUTRA-Bubble can be used for analysis and design of field implementation of IPS by determining injection pressure and duration of a specific concentration of chemical solution to create the desired degree and zone of partial saturation. The extent of the zone of partial saturation is sensitive to the injection pressure, and the final degree of saturation achieved in the zone of partial saturation is a function of the concentration of the chemical solution. The extent of the zone of partial saturation will help to determine the spacing of injection points in the field implementation of IPS.
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# TABLE OF CONTENTS

ABSTRACT .......................................................................................................................... II

LIST OF FIGURES ................................................................................................................ XI

LIST OF TABLES ................................................................................................................ XVI

CHAPTER 1  INTRODUCTION ............................................................................................ 1

CHAPTER 2  LITERATURE REVIEW OF PARTIAL SATURATION ........................................... 5

  2.1  REVIEW OF RESEARCH ON INDUCED PARTIAL SATURATION ............................ 5

  2.2  REVIEW OF PARTIALLY SATURATED SOILS ....................................................... 8

  2.3  REVIEW OF FLOW AND TRANSPORT IN PARTIALLY SATURATED SOILS .......... 12

CHAPTER 3  SUTRA-BUBBLE: MODEL FOR PARTIAL SATURATION
INDUCED THROUGH TRANSPORT AND REACTIVITY .............................................. 18

  3.1  INTRODUCTION TO SUTRA AND SUTRA-BUBBLE ........................................... 18

  3.2  THEORETICAL FORMULATIONS IN SUTRA-BUBBLE .................................... 30

    3.2.1  Degree of Saturation Equation in SUTRA-Bubble ........................................ 30

    3.2.2  Flow Equation in SUTRA-Bubble .................................................................. 33

  3.3  CONSTITUTIVE MODELS IN SUTRA-BUBBLE ..................................................... 36
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3.1 Constitutive Model for Gas Generation in Soil</td>
<td>36</td>
</tr>
<tr>
<td>3.3.2 Constitutive Model for Relative Permeability of Soil</td>
<td>43</td>
</tr>
<tr>
<td>3.4 Fluid Density Model in SUTRA-Bubble</td>
<td>45</td>
</tr>
<tr>
<td>3.5 Modifications of SUTRA Code for SUTRA-Bubble</td>
<td>56</td>
</tr>
<tr>
<td>CHAPTER 4 DETERMINATION OF PARAMETERS FOR CONSTITUTIVE MODELS IN SUTRA-BUBBLE</td>
<td>61</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>61</td>
</tr>
<tr>
<td>4.2 Constitutive Parameters for Gas Generation in Sand</td>
<td>64</td>
</tr>
<tr>
<td>4.2.1 Rate of Gas Generation in Sand</td>
<td>64</td>
</tr>
<tr>
<td>4.2.2 Efficiency of Gas Generation in Sand</td>
<td>70</td>
</tr>
<tr>
<td>4.3 Constitutive Parameter for Relative Permeability of Sand</td>
<td>74</td>
</tr>
<tr>
<td>4.3.1 Laboratory Experiments for Relative Permeability of Sand</td>
<td>74</td>
</tr>
<tr>
<td>CHAPTER 5 VALIDATION OF SUTRA-BUBBLE WITH LABORATORY EXPERIMENTS</td>
<td>80</td>
</tr>
<tr>
<td>5.1 Overview</td>
<td>80</td>
</tr>
<tr>
<td>5.2 Laboratory Experiments</td>
<td>81</td>
</tr>
<tr>
<td>5.2.1 Test Set-up and Procedure</td>
<td>82</td>
</tr>
<tr>
<td>5.2.2 Test Results</td>
<td>98</td>
</tr>
<tr>
<td>5.2.2.1 Test 1 Results</td>
<td>98</td>
</tr>
<tr>
<td>5.2.2.1.1 Flow and Pressure during Injection – TEST 1</td>
<td>98</td>
</tr>
</tbody>
</table>
5.2.2.1.2 Transport of Chemical Solution– TEST 1 ........................................... 102

5.2.2.1.3 Degree of Saturation – TEST 1 .......................................................... 106

5.2.2.2 TEST 2 RESULTS ................................................................................ 114

5.2.2.2.1 Flow and Pressure during Injection – TEST 2 .............................. 114

5.2.2.2.2 Transport of Chemical Solution – TEST 2 ................................... 117

5.2.2.2.3 Degree of Saturation – TEST 2 ....................................................... 119

5.3 SUTRA-BUBBLE SIMULATIONS OF GLASS TANK EXPERIMENTS .......... 125

5.3.1 Preparation of SUTRA-Bubble Simulation .............................................. 127

5.3.2 Back-calculation of Saturated Permeability of Sand Specimen ............... 134

5.3.3 SUTRA-Bubble Outputs ........................................................................... 137

5.3.3.1 OUTPUTS – TEST 1 ............................................................................ 137

5.3.3.2 OUTPUTS – TEST 2 ............................................................................ 142

5.4 COMPARISON OF SUTRA-BUBBLE PREDICTIONS WITH EXPERIMENTAL

RESULTS ........................................................................................................... 145

5.4.1 Comparisons for TEST 1 ......................................................................... 145

5.4.1.1 FLOW AND PRESSURE DURING INJECTION – TEST 1 ................ 145

5.4.1.2 TRANSPORT OF CHEMICAL SOLUTION – TEST 1 ...................... 149

5.4.1.3 DEGREE OF SATURATION – TEST 1 ................................................. 154

5.4.2 Comparison for TEST 2 .......................................................................... 158

5.4.2.1 FLOW AND PRESSURE DURING INJECTION – TEST 2 ................ 158
5.4.2.2 TRANSPORT OF CHEMICAL SOLUTION – TEST 2 ...............................160
5.4.2.3 DEGREE OF SATURATION – TEST 2 ...............................................163
5.4.3 Summary of Comparisons for TEST 1 and TEST 2 ............................166

CHAPTER 6 COMPARISON OF SUTRA-BUBBLE PREDICTIONS WITH
RESULTS OF LARGE SCALE INDUCED PARTIAL SATURATION
EXPERIMENT: LAMINAR BOX ..............................................................168

6.1 OVERVIEW .............................................................................................168
6.2 INDUCED PARTIAL SATURATION EXPERIMENT IN LAMINAR BOX .........169
6.2.1 Laminar Box Experiment .....................................................................169
6.2.2 Degree of Saturation Results from Laminar Box Experiment .............173
6.3 SUTRA-BUBBLE SIMULATION OF LAMINAR BOX SAND SPECIMEN ........177
6.3.1 Determination of Saturated Permeability of Sand Specimen in Laminar
Box ............................................................................................................179
6.3.2 Modeling of Perforated Injection Tube ..................................................183
6.3.3 SUTRA-Bubble Predictions of IPS Experiment in Laminar Box ...........188
6.3.4 Comparison of SUTRA-Bubble Predictions with Experimental Results ...191

CHAPTER 7 SUMMARY AND CONCLUSIONS ............................................196

REFERENCES ..............................................................................................203
LIST OF FIGURES

Figure 2-1 Sketch of a partially saturated soil ................................................................. 9
Figure 2-2 A typical soil-water characteristic curve with various stages of desaturation (Fredlund, 1995) ..................................................................................................................................... 11
Figure 3-1 Sketch describing induced partial saturation (IPS) through transport and reactivity ... 19
Figure 3-2 Schematic for the constitutive model for gas generation in SUTRA-Bubble ............ 37
Figure 3-3 Relative permeability model in SUTRA-Bubble ................................................. 43
Figure 3-4 Schematic showing the fluid density change over the course of the simulation time .. 48
Figure 3-5 Concentration output of SUTRA-Bubble showing the selected locations of Points A, B, and C ............................................................................................................................................. 50
Figure 3-6 BUBSAT subroutine inserted in the main logic of SUTRA ...................................... 59
Figure 4-1 (a) Picture of ASTM graded C778 sand bag (b) Gradation curve for ASTM C778 Ottawa sand (Eseller-Bayat, 2009) .................................................................................................................. 63
Figure 4-2 Batch experiment set-up and electric conductivity meter ........................................ 65
Figure 4-3 Electrical conductivity in sand during gas generation (a) C=0.5% (by weight) and (b) C=1.0% (by weight) ...................................................................................................................... 66
Figure 4-4 Representation of gas bubble generation using electrical conductivity probes .......... 67
Figure 4-5 Fitted equation with exponential rate parameter determined for (a) C=0.5% and (b) C=1.0% .............................................................................................................................................. 69
Figure 4-6 Sketch showing the batch specimen and method to determine Vsource .................... 73
Figure 4-7 The experimental set up for constant head permeability tests ................................. 75
Figure 4-8 Relative permeability of Ottawa sand as a function of degree of saturation .......... 79
Figure 5-1 Sand specimen in glass tank ................................................................................ 81
Figure 5-2 Set-up for IPS experiment in glass tank ............................................................... 82
Figure 5-3 Glass tank and instrumentation and injection tube before specimen preparation ...... 83
Figure 5-4 Fully saturated loose sand specimen prepared in the glass tank ............................. 84
Figure 5-5 Mariotte bottle hanging on the wall supplying constant head flow ....................... 85
Figure 5-6 (a) Picture of the Mariotte bottle (b) Mariotte bottle concept (from, http://en.wikipedia.org/wiki/File:Mariotte_bottle.svg#filelinks ................................................................. 86
Figure 5-7 Sketch of the test for testing the possible head loss in Mariotte bottle set-up ............... 87
Figure 5-8 Pore water pressures measured inside and outside the injection tube ....................... 87
Figure 5-9 Preparation of sodium percarbonate solution .......................................................... 88
Figure 5-10 Measurements of inflow and outflow ................................................................. 89
Figure 5-11 Pore pressure transducers used in laboratory experiments ..................................... 90
Figure 5-12 Electrical conductivity probe and recording meters ............................................ 91
Figure 5-13 Methodology to estimate degree of saturation using Archie’s law ......................... 93
Figure 5-14 Locations of instruments for both Test 1 and Test 2 ............................................ 94
Figure 5-15 Brix probe to measure the dissolved solid concentration at different locations in the sand specimen ....................................................................................................................... 95
Figure 5-16 Digital camera set-up to capture gas bubbles trapped in the sand pores ............... 96
Figure 5-17 Inflow and outflow during (a) water injection and (b) sodium percarbonate solution injection for TEST 1 ................................................................. 99
Figure 5-18 (a) Locations of PPT’s (b) PPT measurements during water injection, (c) PPT measurements during injection of sodium percarbonate solution for TEST 1 ............ 101
Figure 5-19 (a) Locations of electrical conductivity probes (b) Electrical conductivity values measured at 12 probe locations during 13 minute injection of solution for TEST 1 ........ 103
Figure 5-20 Selected results of electrical conductivity (15 minute) superimposed on the picture of the sand specimen ........................................................................................................... 104
Figure 5-21 Electrical conductivity measured during injection and gas generation-TEST 1 ..... 106
Figure 5-22 Selected results of electrical conductivity (12 hours) superimposed on enhanced picture of the sand specimen ........................................................................................................ 108
Figure 5-23 Results for degree of saturation at probes EC1 to EC9 in TEST 1 ......................... 109
Figure 5-24 Picture of partially saturated sand specimen –TEST 1 ........................................... 110
Figure 5-25 Digital images of fully and partially saturated specimens showing gas bubbles for TEST 1 ....................................................................................................................... 111
Figure 5-26 Outflow measured during gas bubble generation - TEST 1 ........................... 112
Figure 5-27 Inflow and outflow during (a) water injection and (b) sodium percarbonate solution injection for TEST 2 .......................................................................................... 115
Figure 5-28 (a) Locations of PPT’s (b) PPT measurements during water injection, (b) PPT measurements during injection of sodium percarbonate solution for TEST 2 ............ 116
Figure 5-29 Locations of electrical conductivity probes (b) Electrical conductivity values measured at 12 probe locations during 13 minute injection of solution for TEST 2 ........ 118
Figure 5-30 Electrical conductivity values measured during injection and gas generation - TEST 2 .................................................................................................................................................. 120
Figure 5-31 Results for degree of saturation at probes EC1 through EC9 – TEST 2 ............... 121
Figure 5-32 Picture of partially saturated sand specimen – TEST 2 ........................................ 121
Figure 5-33 Digital images of fully and partially saturated specimens showing gas bubbles for
TEST 2 ................................................................................................................................. 122
Figure 5-34 Outflow measured during gas bubble generation - TEST 2 ................................. 124
Figure 5-35 Steps for validation of SUTRA-Bubble predictions ............................................. 126
Figure 5-36 SUTRA-Bubble mesh for Glass Tank experiment set up (a) 3-D view of the mesh (b)
elevation view of the mesh ................................................................................................. 128
Figure 5-37 Soil elements at the injection tube location .......................................................... 129
Figure 5-38 Concept of impermeable zone for injection tube (a) elevation (b) plan................. 130
Figure 5-39 Input flow of clean water and SUTRA-Bubble prediction at injection nodes (a) TEST
1 (b) TEST 2 ....................................................................................................................... 135
Figure 5-40 (a) Locations for pore pressure transducers; Comparison of predicted and measured
pressures (b) for TEST 1 (c) for TEST 2 ................................................................................ 136
Figure 5-41 Section A-A, B-B, and C-C of the SUTRA-Bubble mesh ........................................ 137
Figure 5-42 Concentration outputs of SUTRA-Bubble simulation for TEST 1 at 15 minutes after
injection (a) 3-D view (b) Section C-C (c) Section A-A (d) Section B-B ............................ 138
Figure 5-43 Degree of saturation outputs of SUTRA-Bubble simulation for TEST 1 (a) Section C-
C (b) Section A-A (c) Section B-B ..................................................................................... 141
Figure 5-44 Degree of saturation output of SUTRA-Bubble simulation for TEST 1 for Section D-
D .......................................................................................................................................... 141
Figure 5-45 Concentration outputs of SUTRA-Bubble simulation for TEST 2 at 15 minutes after
injection (a) 3-D view (b) Section A-A (c) Section B-B......................................................... 143
Figure 5-46 Degree of saturation outputs of SUTRA-Bubble simulation for TEST 2 (a) Section C-
C (b) Section A-A (c) Section B-B ..................................................................................... 144
Figure 5-47 Inflow assigned for 13 minutes in SUTRA-Bubble simulation of TEST 1 ............... 146
Figure 5-48 Inflow and outflow values computed by SUTRA-Bubble for TEST 1 compared with
measured data ...................................................................................................................... 147
Figure 5-49 Comparison for predicted and measured pressures for TEST 1 ............................ 148
Figure 5-50 Concentration output of SUTRA-Bubble for TEST 1 with superimposed locations of
electric conductivity probes .............................................................................................. 149
Figure 5-51 (a) Locations of electrical conductivity probes (b) breakthrough curve at probes EC1 and EC2 (c) breakthrough curve at probes EC3, EC5, and EC6 ......................................................... 152
Figure 5-52 (a) Breakthrough curve at probe EC7 (b) breakthrough curve at probes EC4 and EC9 (c) breakthrough curve at probe EC8 ............................................................................................. 153
Figure 5-53 Degree of saturation output of SUTRA-Bubble for TEST 1 with superimposed locations of electric conductivity probes ........................................................................................................ 154
Figure 5-54 Comparison of predicted and measured degree of saturation for TEST 1 ............. 156
Figure 5-55 Comparison of predicted and measured outflow of solution for TEST 1 ............ 157
Figure 5-56 Inflow assigned for 13 minutes in SUTRA-Bubble simulation of TEST 2 .......... 158
Figure 5-57 Inflow and outflow values computed by SUTRA-Bubble for TEST 2 compared with measured data .......................................................................................................................... 159
Figure 5-58 Comparison for predicted and measured pressures for TEST 2 ....................... 160
Figure 5-59 Concentration output of SUTRA-Bubble for TEST 2 with superimposed locations of electric conductivity probes .................................................................................................................. 161
Figure 5-60 Breakthrough curves at probes (a) EC1 and EC2 (b) EC3, EC5, and EC6 (c) EC7 and (d) EC4 and EC9 - TEST 2 ................................................................................................................. 162
Figure 5-61 Breakthrough curve at probe EC8 – TEST 2 .................................................................................. 163
Figure 5-62 Degree of saturation output of SUTRA-Bubble for TEST 2 with superimposed locations of electric conductivity probes ........................................................................................................ 164
Figure 5-63 Comparison of predicted and measured degree of saturation for TEST 2 ............ 165
Figure 5-64 Comparison of predicted and measured outflow of solution for TEST 2 .......... 166
Figure 6-1(a) 2-story tall Laminar Box IPS set-up (b) top of a sand specimen ...................... 170
Figure 6-2 IPS system and injection tube used in the Laminar Box experiments .................... 171
Figure 6-3 Locations of 31 injections performed for treating the bottom and top of the sand specimen in the Laminar Box ............................................................................................................. 172
Figure 6-4 Typical electrical conductivity probe with a long cables, inserted in the laminar box specimen .................................................................................................................................................. 173
Figure 6-5 Instruments in the area for planned simulation of Injection 1 (a) plan (b) elevation . 174
Figure 6-6 Degree of saturation at each probe location within the planned simulation area...... 175
Figure 6-7 Zone of partial saturation around Injection 1 in plan view of the box .................... 176
Figure 6-8 Portion of the sand specimen simulated in SUTRA-Bubble .................................. 177
Figure 6-9 3D SUTRA-Bubble mesh of the simulated portion of the Laminar Box ............... 178
Figure 6-10 Experimental set-up for water injection test in the Laminar Box ....................... 180
Figure 6-11 SUTRA-Bubble mesh for flow rate test in the Laminar Box .................................. 181
Figure 6-12 Permeability of sand specimen in the Laminar Box .................................................. 182
Figure 6-13 Modeling of perforated injection tube ....................................................................... 184
Figure 6-14 Plan view of SUTRA-Bubble mesh showing the injection tip opening .................... 185
Figure 6-15 SUTRA-Bubble mesh of IPS experiment in the Laminar Box (a) 3D (b) elevation 186
Figure 6-16 The three sections used to present SUTRA-Bubble predictions (a) Section A-A and
B-B in elevation and (b)Section C-C in plan ............................................................................. 188
Figure 6-17 Concentration output of SUTRA-Bubble for Section A-A during injection process (5
lifts - each 1ft) ...................................................................................................................... 189
Figure 6-18 Degree of saturation output of SUTRA-Bubble for Section A-A .............................. 190
Figure 6-19 Degree of saturation output of SUTRA-Bubble for Section C-C ............................... 191
Figure 6-20 Comparison of SUTRA-Bubble predictions for degree of saturation with conductivity
probe measurements (a) Section A-A (b) Section B-B ......................................................... 193
Figure 6-21 Comparison of partial saturation zones determined using conductivity probes and
SUTRA-Bubble predictions ...................................................................................................... 194
LIST OF TABLES

Table 3-1 Constant values used in SUTRA-Bubble source code .................................................. 60
Table 4-1 Goodness of fit test results for exponential rate parameter ........................................... 70
Table 4-2 Loss due to solubility of oxygen gas under normal conditions ...................................... 71
Table 4-3 Bench top experiment output to determine efficiency of sodium percarbonate reaction in sand .......................................................................................................................... 73
Table 4-4 Results of constant head permeability tests ................................................................. 76
Table 4-5 Average saturated permeability values, kFS in Equation (4-3) corrected for void ratio 77
Table 4-6 Relative permeability values ......................................................................................... 78
Table 5-1 Parameters of injection of sodium percarbonate solution in glass tank experiments .... 97
Table 5-2 Brix probe measurements of sodium percarbonate concentration for TEST 1 ........... 106
Table 5-3 Brix probe measurements of sodium percarbonate concentrations –TEST 2 .......... 119
Table 5-4 Input concentration values used in SUTRA-Bubble simulation .................................. 131
Table 5-5 Summary of parameters used in SUTRA-Bubble simulation ...................................... 133
Table 5-6 Validation of SUTRA-Bubble with Glass Tank IPS Experimental Tests ................... 167
Table 6-1 Laboratory data for permeability for F55 Ottawa sand ............................................... 179
Table 6-2 Measured data for flow rate test in Laminar Box ........................................................ 180
Table 6-3 List of input parameters used in SUTRA-Bubble simulation of IPS experiment in the Laminar Box ........................................................................................................................ 187
Table 6-4 Predicted and measured degree of saturation values at each probe location .......... 194
Table 6-5 Validation of SUTRA-Bubble with the Laminar Box IPS Experimental Test .......... 195
Table 7-1 Validation of SUTRA-Bubble with Glass Tank IPS Experimental Tests ................... 201
Table 7-2 Validation of SUTRA-Bubble with the Laminar Box IPS Experimental Test .......... 202
Chapter 1

Introduction

Liquefaction of loose saturated sands during an earthquake can lead to significant damage to the built environment. There are a number of liquefaction mitigation measures available in practice such as vertical drains, in-situ densification, and grouting. During the past decade, new liquefaction mitigation measures have been investigated by a number of researchers. These techniques include; desaturation through pumping air (Shiraishi, 2007 and Okamura, 2011), biogenic gas generation (Rebata-Landa, 2007), bio cementation (DeJong et al. 2006), colloidal silica grouting (Gallagher et al. 2007, Gallagher and Lin, 2009), electro-osmosis gradient application (Hocking, 2003), and inducing partial saturation in situ by generation of gas bubbles (Yegian et al. 2007).

An innovative liquefaction mitigation technique called Induced Partial Saturation (IPS) in sands has been introduced by Yegian et al. (2007), and Eseller-Bayat et al. (2013). The technique involves creating gas bubbles in the pore spaces of a sand skeleton, thus creating partial saturation without disturbing the in-situ stress conditions. The benefit of this technique on liquefaction resistance of sands was shown in results from shaking table experiments presented by Yegian et al. (2007), and Eseller-Bayat et al. (2013).

Recent research at Northeastern University focuses on developing a field method to implement the Induced Partial Saturation technique. The field method involves injection of a chemical solution into a liquefaction-susceptible fully saturated sand deposit without disturbing in-situ stress conditions. The chemical solution is injected and transported under controlled pressure and in time generates gas bubbles. The gas bubbles generated
throughout the transport of the chemical solution are trapped in the pores of the sand and hence increase the compressibility of the soil by creating partial saturation. The research reported in this dissertation investigates the use of sodium percarbonate as the chemical that dissolves in water, and through transport generates oxygen gas bubbles within the pores of fully saturated sand.

The research presented in this dissertation addresses the need for a numerical simulation tool that can be used to design the delivery system for IPS implementation in the field. The design parameters for the delivery system include: 1) injection pressure and duration for creating a certain zone of partial saturation, 2) concentration of sodium percarbonate solution to achieve a certain level of partial saturation, and 3) zone of partial saturation created, which determines the design spacing of injection points. The numerical simulation technique can then be used to optimize the design parameters of the delivery system for full-scale field applications. The objective of this research was to develop a computer software that can perform numerical modelling in three-dimensions (3D) for transport and chemical reactivity of sodium percarbonate solution in fully saturated sand, leading to reduction in degree of saturation.

To simulate partial saturation induced through transport and reactivity of sodium percarbonate solution, modifications were made in the program called “SUTRA (Saturated- Unsaturated Transport) is a computer program that simulates fluid movement and the transport of either energy or dissolved substances in a subsurface environment (Voss and Provost, 2010)” SUTRA models flow through fully and partially saturated soils where partial saturation is due to capillarity above a fully saturated region. This condition of unsaturation is different from the partial saturation created by IPS technique. IPS
transforms a fully saturated sand into a partially saturated by generating gas bubbles in sand pores below the water table. In this situation the water pressure remains above atmospheric but compressibility of the sand, water, gas matrix is reduced. A modified version of SUTRA was needed to simulate partial saturation created by the IPS technique. SUTRA-Bubble is this modified version of SUTRA that can simulate the transport of a chemical solution and its reactivity, thus generating gas bubbles leading to partial saturation and reduction in permeability in sands and an increase in the effective fluid compressibility. It is noted that this reduction in permeability also impacts the transport of the chemical solution, which SUTRA-Bubble incorporates.

This dissertation presents the details of the theoretical formulations and their incorporation in the numerical simulation program. It also includes details and results from laboratory experiments on small-scale implementation of IPS to validate SUTRA-Bubble.

Chapter 2 presents a review of partial saturation created by the IPS technique and by capillarity. The chapter also discusses the fundamentals of flow and transport in partially saturated soils.

Chapter 3 introduces SUTRA-Bubble as a modified version of SUTRA. In this chapter, the theoretical formulation of SUTRA-Bubble is presented, which involves coupling the ideal gas law with the fluid mass balance equation for flow. The chapter also presents two constitutive models to solve for the time-dependent generation of gas bubbles and the reduction in soil permeability due to induced partial saturation.

Chapter 4 presents laboratory experiments conducted to determine the parameters for the two constitutive models in SUTRA-Bubble, including: 1) rate of generation of gas
bubbles as a function of chemical concentration, and 2) reduction in soil permeability due to partial saturation.

Chapter 5 presents laboratory experiments performed to validate SUTRA-Bubble. The chapter describes implementation of IPS in a large sand specimen prepared in a specially manufactured glass tank. The predictions made by SUTRA-Bubble in terms of measured pore pressures, flow rate, zone of partial saturation, and degree of saturation were compared with the test results for the purpose of validation of the developed numerical simulation.

In Chapter 6, comparisons are made between SUTRA-Bubble predictions and selected results from a large-scale implementation of IPS in the Laminar Box at the State University of Buffalo (NEES @ Buffalo site), again for the purpose of validation.

Finally, Chapter 7 presents a summary of the research work presented in this dissertation, followed by conclusions made based on the theoretical and experimental research results.
Chapter 2

Literature Review of Partial Saturation

This chapter presents literature review of partially saturated sands. Section 2.1 focuses on sands that are partially saturated by the Induced Partial Saturation (IPS) Technique. Section 2.2 briefly discusses sands that are partially saturated by capillarity. The differences between sands partially saturated by IPS or capillarity are discussed. It is noted that research reported in this dissertation focuses on sands that are partially saturated by IPS. Section 2.3 briefly reviews modeling approaches for flow and transport in partially saturated soils.

2.1 Review of Research on Induced Partial Saturation

The Induced Partial Saturation (IPS) technique for liquefaction mitigation was developed and investigated by researchers at Northeastern University. The benefit of IPS as a liquefaction mitigation measure has been demonstrated by (Yegian et al. (2007) and Eseller-Bayat et al. (2013)). Different techniques have been employed to create partial saturation in sands in the laboratory including: electrolysis, drainage and recharge of pore water, and dissolved Efferdent® chemical powder. The results published by Yegian et al. (2007) described two different methods to prepare partially saturated specimens. The first method involved electrolysis of the pore water utilizing two electrodes. This method was able to create any degree of partial saturation in a sand specimen by adjusting the current. However, the gas generation was limited to the region around the electrodes. The drainage-recharge method involved draining pore water out of a fully saturated specimen and recharging the specimen from the top to trap air in the void space of the sand. This method
was able to create partially saturated specimens, but the degree of saturation was limited to \( S = 82\% \) to 86\%. The continuation of this work published recently by Eseller-Bayat et al. (2013) presented another method to prepare partially saturated specimens with various degrees of saturation. The method utilized a commercially available dental product in a tablet form called Efferdent, which generates oxygen gas by its reaction with water. The main component of Efferdent is sodium perborate which has a chemical reaction as follows (Eseller-Bayat et al. 2013):

\[
2(\text{NaBO}_3\cdot\text{H}_2\text{O}) + 2\text{H}_2\text{O} \rightarrow 2\text{H}_2\text{O}_2 + 2\text{BO}_3^{3-} + 2\text{Na}^+ + 4\text{H}^+
\]

\[
2\text{H}_2\text{O}_2 \rightarrow 2\text{H}_2\text{O} + \text{O}_2
\]

Sodium perborate dissolves in water and creates hydrogen peroxide along with several ions. Hydrogen peroxide in solution creates oxygen gas bubbles. It was noted from the experiment that the oxygen gas generation was quite fast, which caused most of the oxygen gas bubbles to escape into the atmosphere. The most effective way to minimize the loss in volume of oxygen gas bubbles was to mix the dry sand with powdered Efferdent® with a certain mass fraction before sample preparation. Partially saturated specimens were then prepared by a wet pluviation technique in which the mixture of dry sand and powdered Efferdent was rained into water. Different mass fractions of Efferdent and dry sand led to different degrees of saturation in the specimen. The details of the sample preparation are included in published thesis by Eseller-Bayat, 2009 and Gokyer, 2009. Results from a number of shake table tests published in Eseller-Bayat et al. (2013), demonstrated the benefit of IPS as a liquefaction mitigation measure.
The three partially saturated sample preparation methods described were effective in laboratory applications, but it was concluded that their use in the field would not be practical. Recent research at Northeastern University focuses on a field method for inducing partial saturation by injecting a gas-generating chemical solution into a fully saturated portion of a sand deposit, and as gas bubbles are generated within the pores of the sand, the degree of saturation is reduced. In order to achieve a practical zone of partial saturation through injection of a chemical solution, the gas generation should be slow enough to allow transport of solution without bubble clogging. Sodium percarbonate was found to be ideal because of its slow rate of gas generating reaction in water. Sodium percarbonate dissolves in water and dissociates into sodium and carbonate ions, as well as hydrogen peroxide, which is the source of oxygen gas bubbles, as shown below in the associated chemical reactions.

\[
\begin{align*}
\text{Na}_2\text{CO}_3 \cdot 1.5\text{H}_2\text{O}_2 \quad \text{in water} & \quad \rightarrow 2\text{Na}^{+1} + \text{CO}_3^{2-} + 1.5\text{H}_2\text{O}_2 \\
1.5\text{H}_2\text{O}_2 \quad \text{in water} & \quad \rightarrow 1.5\text{H}_2\text{O} + 0.75\text{O}_2
\end{align*}
\]

(at the end of reaction)

(ideal conditions - 100% efficiency)

There are other uses of the sodium percarbonate that was used for generation of oxygen gas. Sodium percarbonate is a primary component in household cleaning agents and it is preferred for its environmental safety. For instance, sodium percarbonate is the main ingredient in OxiCleanTM which is widely used as a cleaning agent. Moreover, injection of sodium percarbonate solution has been used commercially by many companies such as Regenesis and EnviroFIRST as an in-situ chemical oxidation technique for geo-environmental remediation. These companies have stated that sodium percarbonate is environmentally friendly and easy to apply to the contaminated subsurface without health
and safety concerns. Sodium percarbonate is also used in bioremediation to eliminate organic contaminants (Vesper et al. 1994).

Sodium percarbonate is a white crystalline powder. It dissolves in water with a solubility of 140 g/l at 20 °C. The solution of sodium percarbonate is basic with a pH of 10.5 at 1% concentration at 20 °C. Injection of sodium percarbonate solution into the ground will increase the pH of the ambient groundwater. However, Regenesis states that four (4) weeks after injection the pH returns to its original ambient level (Regenesis, 2007).

As a result of these investigations, sodium percarbonate was selected as the source for gas generation for implementing Induced Partial Saturation in the field.

A delivery system was designed for inducing partial saturation through injection of a chemical solution and its transport and reactivity in sand. The system is being patented by Professors Yegian and Alshawabkeh through Northeastern University.

The research presented in this dissertation is part of a large project on IPS funded by the Network for Earthquake Engineering Simulation (NEES) of the National Science Foundation (NSF). This dissertation focuses on the numerical simulation of transport and reactivity of sodium percarbonate solution for inducing partial saturation in order to be able to design the optimal IPS delivery system in the field.

2.2 Review of Partially Saturated Soils

The behavior of partially saturated soils is more complex than fully saturated soils, due to their three phase micro structure including solid skeleton, pore fluid (water), and gas/air (Figure 2-1).
The behavior of partially saturated soils may differ depending on the degree of saturation. Volume of the gas/air bubbles compared to the pore space or solid particles lead to different mechanisms in the micro structure of a soil. Therefore, different types of partially saturated soils are defined at various degrees of saturation with different mechanical structures. There have been many researchers investigating the mechanical behavior of different types of partially saturated soils. Fredlund and Rahardjo (1993) divided the partially saturated soils into three types as a function of degree of saturation. The first type is a partially saturated soil with a degree of saturation less than approximately 80%. In this type, the gas phase is continuous and menisci of pore fluid adhere to the solid grains. The second type is a partially saturated soil with degree of saturation in between 80% to 90%. In this type there is a transition state where the air phase is still continuous and liquid phase is also continuous with occluded bubbles. The third type is a partially saturated soil with degree of saturation greater than 90%. In this type, the gas phase is all in occluded form and pore fluid is continuous. In addition to these three types, Pietruszczak and Pande (1996) stated that there is another form of partial saturation called “gassy soil”. In this type of partially saturated soil, the gas phase is discontinuous in the form of discrete occluded bubbles that are entrapped in void space of soil deposit. They also reported that
in this type of structure, gas is formed through the decomposition of organic matter and the gas formed becomes much larger than the average particle size, thus pushing against the soil skeleton. Naturally occurring gassy soils are mainly observed in marine sediments. Wheeler, (1988) stated that since in gassy soils the gas bubbles are much larger than the normal void space, they cannot be considered as occluded bubbles within the pore water. The gas bubbles generated in IPS technique are smaller than the void space since the gas generation is finite and limited by the duration of the chemical reaction of sodium percarbonate. A partially saturated soil created by IPS does not fit in any of these types, where occluded gas bubbles are entrapped in void space of sand in a size smaller than void space. The effect of these gas bubbles on the soil structure is simply changing the compressibility of the pore fluid, which is the benefit of the method regarding liquefaction mitigation.

The types of partially saturated soils different from IPS described above appear all in the zone above the water table where capillary pressures appear. This capillary pressure is also known as matric suction. Matric suction is the pressure difference between air pressure and water pressure. Since most of the time the air phase is continuous in the capillary zone, the matric suction appears as a negative pore pressure in the pore space for this type of partially saturated soils. The type of partially saturated soil is described by a soil-water characteristic curve which relates the matric suction of the soil to the degree of saturation as shown in Figure 2-2 (Fredlund, 1995).
However, in applications of IPS, partial saturation is created below the water table where pore water pressure is positive. Moreover, the gas bubbles stay occluded and smaller than the pore space, which means the pore water stays continuous in the pore space. For this reason, in the IPS type of partially saturated soils pore water pressures are above atmospheric, as was also stated by Pietruszczak and Pande (1996).

The pressure of gas bubbles in a pore space to pore water pressure through Equation 2-1 which is referred to as Kelvin’s capillary model equation (Fredlund and Rahardjo, 1993):

\[
(u_a - u_w) = \frac{2T_s}{R_s}
\]  

(2-1)

where

- \(u_a\) = air pressure
- \(u_w\) = water pressure
- \(T_s\) = surface tension
- \(R_s\) = radius of curvature
In the case of occluded bubbles, Fredlund and Rahardjo, (1993) and Bishop and Eldin, (1950) suggested to neglect the effect of surface tension ( ). At this stage, for the type of partially saturated soils created by IPS, the air pressure in the pore space ( ) is assumed to be equal to the pore water pressure ( ) which is above atmospheric pressure all the time. Measured pore water pressures in the laboratory experiments conducted to show the benefit of IPS technique were positive as published by Eseller-Bayat et al. (2013). The validity of this simplification in field application of IPS technique can be investigated in the future.

It is also known that the permeability of partially saturated sands is different from that of fully saturated sands. There are a number of studies that have related permeability of partially saturated sands to those of fully saturated sands. The available empirical relationships in the literature are presented in Section 3.3.2. The section also describes the constitutive model for relative permeability (reduced permeability of partially saturated soil relative to permeability of fully saturated soil) that was implemented in SUTRA-Bubble.

**2.3 Review of Flow and Transport in Partially Saturated Soils**

Simulation of IPS through flow and transport of sodium percarbonate solution can be modeled with the coupled flow of pore fluid with variable density into saturated and unsaturated soils and transport of dissolved species. Sodium percarbonate dissociates in water into sodium and carbonate ions and hydrogen peroxide, which generates oxygen gas through its decomposition in water. The transport and reactivity of hydrogen peroxide as a solute in water generates gas bubbles trapped in sand pores leading to partial saturation.
in sand. Moreover, the solution of sodium percarbonate increases the fluid density depending on its concentration.

Flow in partially saturated soils has been studied by many researchers to understand infiltration and recharge (by precipitation, irrigation, or artificial recharge) and movement of pollutants with infiltration caused by landfills, fertilizers, etc. (Bear, 1979). Therefore, studies of flow and transport in partially saturated soil are restricted to the capillary zone above the water table.

Flow through saturated porous media is governed by Darcy’s law. Darcy’s law also applies for flow through partially saturated soils (Fredlund and Rahardjo, 1993). However, as mentioned earlier, in partially saturated soils the coefficient of permeability is not the same as in fully saturated soils, and it may change during the flow. The governing equation of flow in an unsaturated zone is derived by combining Darcy’s velocity equation with mass conservation of the pore water (Bear, 1979). Simulation methods for flow of fluid in an unsaturated zone are all based on this governing equation.

Transport of dissolved species are modeled with advection, dispersion, and diffusion mechanisms as well as with reactivity, if applicable. Advection is the transport of solute along with the pore fluid flowing due to a hydraulic gradient. Advection leads to transport of solute with an average rate equal to the seepage velocity of the pore fluid, if the solute is non-reactive.

\[ J_{\text{advection}} = n v C \]  

(2-2)

where:

\[ J_{\text{advection}} = \text{mass of solute flowing per unit area per unit time due to advection} \]
\[ n = \text{porosity} \]
\[ \nu_s = \text{seepage velocity} \]
\[ C = \text{concentration of solute} \]

Dispersion is the spreading of the solute concentration, which is attributed to the variations in seepage velocity. The main mechanisms leading to dispersion are stated as variability in size of pore space within soil, variations in tortuosity, and permeability of soil, and variability in flow velocity across any cross section within soil (Fried, 1975; Bear, 1979; Freeze and Cherry, 1979). Dispersivity is determined in laboratory tests to vary from 0.0001 to 0.01 mm (Gillham and Cherry, 1982) and in field measurements from 1 to 100 m (Mohamed and Antia, 1998). Dispersivity is a scale dependent parameter where it can also be greater than 100 m for regional-scale problems. This variability is attributed to the heterogeneities in soils under field conditions.

\[ J_{\text{dispersion}} = - n \alpha_1 \nu_s \frac{\partial C}{\partial x} \]  

(2-3)

where:
\[ J_{\text{dispersion}} = \text{mass of solute flowing per unit area per unit time with dispersion} \]
\[ n = \text{porosity} \]
\[ \alpha_1 = \text{longitudinal dispersivity} \]
\[ \nu_s = \text{seepage velocity} \]
\[ C = \text{concentration of solute} \]

Equation (2-3) represents 1D dispersion relation which is simplified to longitudinal dispersivity. For 2D or 3D dispersion, both longitudinal and transverse dispersion should be taken into account.
Diffusion is the migration of the solute at the molecular level due to distance concentration gradient. Diffusion of solute in a porous medium depends on soil porosity and tortuosity together with diffusion coefficient of ions. Diffusion coefficients for sodium (Na+) and carbonate (CO3-2) are 13.3 E-10 m2/sec and 9.55 E-10 m2/sec, respectively at 25 °C (Mohamed and Antia, 1998). In coarse grained soils where the fluid velocities are fast, the rate of diffusion is very small relative to fluid velocities. Therefore, the effect of diffusion of solute compared to advection and dispersion is insignificant. Equation (2-4) below presents 1D diffusion in soils.

\[
J_{\text{diffusion}} = -D_0 \tau n \frac{\partial C}{\partial x}
\]

(2-4)

where:

\[J_{\text{diffusion}} = \text{mass of solute flowing per unit area per unit time with diffusion}\]

\[n = \text{porosity}\]

\[\tau = \text{tortuosity of soil}\]

\[C = \text{concentration of solute}\]

Reactivity of solute in pore fluid leads to decomposition of solute concentration as a function of time. Transport of sodium percarbonate solution in sand for implementation of IPS includes all these four mechanisms; advection, dispersion, diffusion, and reactivity.

\[
J_{\text{reactivity}} = -rC
\]

(2-5)

where:

\[J_{\text{reactivity}} = \text{mass of solute flowing per unit area per unit time with reactivity}\]
\[ r = \text{rate of decomposition of solute in fluid} \]
\[ C = \text{concentration of solute} \]

The governing equation for transport of solute concentration is the conservation of the solute mass, which includes the four mechanisms described above.

In addition, as was mentioned above, dissolved sodium percarbonate in water increases the fluid density proportional to its concentration. Therefore, flow and transport processes should be coupled. There are numerical modeling approaches for flow and transport of variable density pore fluid in saturated and unsaturated zones. The governing equations for these models are: Darcy’s law with fluid density, fluid mass balance equation (conservation of fluid mass), and mass balance for solute (conservation of solute mass). In these governing equations, density of pore fluid is related to the concentration of solute, and the relative permeability is a function of the degree of saturation. There are numerical simulators available for modeling variable density flow and transport in saturated and unsaturated soils such as DEDALE created by Usseglio-Polatera et al. (1990), and SUTRA by Voss, (1984).

In this research, SUTRA was modified to solve for the flow and transport as well as reactivity components of IPS. SUTRA uses a relative permeability coefficient in Darcy’s velocity equation for simulating flow in partially saturated soils, which can be user defined as a desired function of either degree of saturation or capillary pressure. This flexibility in SUTRA enabled the elimination of capillary pressures and relating relative permeability directly to degree of saturation, for IPS application. In addition, the capability of SUTRA to relate the degree of saturation to the reactivity of the solute in pore fluid (sodium percarbonate in water) was also utilized.
The next chapter presents SUTRA-Bubble, which is the modified version of SUTRA. SUTRA-Bubble is used as a tool for simulation of inducing partial saturation in sands through transport and reactivity for liquefaction mitigation.
Chapter 3

SUTRA-Bubble: Model for Partial Saturation Induced through Transport and Reactivity

3.1 Introduction to SUTRA and SUTRA-Bubble

Field implementation of IPS involves injection of sodium percarbonate solution into saturated sand with controlled pressure and concentration. The reactivity of the sodium percarbonate solution during its transport in sand leads to generation of gas bubbles entrapped in the pore space, thus inducing partial saturation within a certain zone (Figure 3-1). In order to design an IPS field implementation program, a numerical simulation tool is needed to help define the various design parameters including: injection pressure and duration for creating a certain zone of partial saturation; concentration of sodium percarbonate solution to achieve a certain level of partial saturation; and zone of partial saturation created, which determines the design spacing of injection points. To achieve this goal, a modified version of SUTRA was developed. The modified program SUTRA-Bubble can model partial saturation induced through transport and reactivity of a chemical solution.
Figure 3-1 Sketch describing induced partial saturation (IPS) through transport and reactivity

The computer program SUTRA-Bubble can model 3D flow and reactivity accounting time-dependent reduction in degree of saturation and permeability as well as effect of variable fluid density.

The computer program SUTRA was originally developed by Voss in 1984 and updated latest (SUTRA 2.2) by Voss and Provost in 2010. “SUTRA (Saturated-Unsaturated Transport) is a computer program that simulates fluid movement and the transport of either energy or dissolved substances in a subsurface environment (Voss and Provost, 2010)”. 

In regards to simulation of induced partial saturation, saturated or unsaturated density dependent flow and transport of a solute with decay are the essential processes that need to be formulated. SUTRA allows modeling of two interdependent processes; fluid density
dependent saturated or unsaturated flow and transport of a solute subject to reactivity (exponential decay). Moreover, the modular design of the code to solve for its governing equations allows modifications to the code both in fluid movement and the transport processes. This modularized structure of the code enabled the specific modifications needed both in partially saturated flow and in coupling of transport of solute with partial saturation that are needed to simulate implementation of induced partial saturation.

SUTRA uses a combination of finite-element and finite-difference methods to approximate the governing equations for flow and transport both for 2D and 3D simulations of a subsurface environment. The program is robust and accurate with proper spatial and time discretization. The details of the numerical methods employed in SUTRA are described by Voss and Provost, (2010).

SUTRA calculates fluid pressures, solute concentrations, and degrees of saturation as functions of time. SUTRA code recognizes the partially saturated zone above the water table where capillary pressures appear, as most of the types of partially saturated soil observed in the field are in the capillary zone with various degrees of saturation. As also described in Section 2.2 in detail, since most of the time the air phase is continuous and connected to the atmosphere, the capillary pressure appears as a negative pore pressure in the pore space for this type of partially saturated soils. It should be noted that the fluid pressure calculated in SUTRA is gauge pressure that is relative to atmospheric. If the pressure drops below zero (below atmospheric) due to the difference between air and water pressures in the pore space (surface tension effect between the air, the pore fluid, and the solid grains), that negative pressure is recognized as capillary pressure in SUTRA to activate its unsaturated model. Capillary pressure is related to pore pressure by:
\[ p_c = \begin{cases} -p & \text{when } p < 0 \\ 0 & \text{when } p \geq 0 \end{cases} \] (3-1)

where:

- \( p_c \) = capillary pressure
- \( p \) = fluid pressure

According to the mechanics of a capillary zone, when the critical capillary pressure is achieved for air entry into the pores, air enters the pore space of the soil and water saturation in the pores decreases to create partially saturated conditions. Therefore, the degree of saturation in this capillary zone is related to the capillary pressure. This relation is determined empirically by laboratory experiments on different types of soils. SUTRA does not limit the use to a particular relationship but suggests and includes the function published by van Genuchten, (1980) in the code, which is shown in Equation (3-2). The equation shows that when the capillary pressure is zero, the degree of saturation is equal to 1.0.

\[ S_w = S_{w_{res}} + (1 - S_{w_{res}}) \left[ \frac{1}{1 + (a p_c)^n} \right]^{(n+1)/n} \] (3-2)

where:

- \( S_w \) = degree of saturation
- \( S_{w_{res}} \) = residual degree of saturation (below which saturation is not expected to fall)
- \( p_c \) = capillary pressure
- \( a \) and \( n \) = parameters chosen for different types of soils
The type of partial saturation created by IPS is different from naturally occurring partial saturation resulting from dessication or movement of the phreatic line as explained in Chapter 2-2. Partial saturation created by IPS is in pores below the water table, which are saturated before injection is applied. The generated gas bubbles are in an occluded state and smaller than the void space, and the pore fluid in the void space is continuous. The gas bubbles are connected to the atmosphere through the pore fluid. The surface tension is neglected in this type of partial saturation and thus the pore pressure is equal to the pressure of the pore fluid. For this reason, the pore fluid pressure is always above atmospheric (positive gauge fluid pressure). Therefore, it was determined that modifications to the SUTRA code needed to be done under the saturated mode where fluid pressures are always positive.

SUTRA-Bubble, was developed to simulate this new partial saturation created through transport and reactivity of a solute. A new relationship to calculate the degree of saturation is developed in SUTRA-Bubble.

Later in this chapter, the modifications introduced in SUTRA in order to create SUTRA-Bubble, using a new relationship for degree of saturation, is presented in detail. In order to understand the added formulations in SUTRA-Bubble, the flow model used in SUTRA is described below.

**Saturated- Unsaturated Ground-Water Flow simulation in SUTRA**

SUTRA simulates flow in porous media using mass conservation of pore fluid. The total mass of fluid in the pore space of the solid matrix might change with time due to hydraulic flow created by injection or extraction wells, changes in fluid density caused by dissolved solids in pore fluid, and changes in the degree of saturation. The governing
equation for flow simulation in SUTRA is a fluid mass-balance equation that keeps track of the change in fluid mass contained everywhere in the simulated subsurface environment with time due to any source of flow. The fluid mass balance equation is expressed as the sum of pure water and pure solute mass balances for a solid matrix by Voss and Provost, (2010) as shown in Equation (3-3). The program assumes no subsidence or compaction built into this equation.

\[
\frac{\partial (\varepsilon S_w \rho)}{\partial t} = -\nabla (\varepsilon S_w \rho \mathbf{v}) + Q_p + Y
\]

(3-3)

where:
\[\varepsilon = \text{porosity of soil}\]
\[S_w = \text{degree of saturation of soil}\]
\[\rho = \text{density of soil}\]
\[\mathbf{v} = \text{fluid velocity}\]
\[Q_p = \text{fluid mass source (including pure water mass plus solute dissolved in source water)}\]
\[Y = \text{solute mass source (e.g. dissolution of solid matrix or desorption)}\]

In Equation 3-3, the term \((\varepsilon S_w \rho)\) is the total fluid mass unit volume, and the term on the left side of the Equation (3-3), \(\frac{\partial (\varepsilon S_w \rho)}{\partial t}\), is the rate of change in total fluid mass contained in the void space. The term on the right side of the equation \(-\nabla \cdot (\varepsilon S_w \rho \mathbf{v})\) is the local change in fluid mass entering the void space as a result of the difference between fluid inflows and outflows in a unit volume. \(Q_p\) is the external source of fluid which includes the pure water and dissolved solids. \(Y\) is the pure solute mass not associated with a fluid source. Since the contribution of \(Y\) to the solute mass is typically small, it is neglected in SUTRA. This fundamental relationship for mass-balance of fluid needs to be
expressed in terms of the primary variables, fluid pressure \(p\), and solute concentration \(C\).

Fluid velocity, \(\bar{v}\) in Equation (3-3) is described by Darcy’s law as shown in Equation (3-4) where fluid density is variable.

\[
\bar{v} = - \left( \frac{k r}{\varepsilon S_w \mu} \right) \cdot (\nabla p - \rho g)
\]

where:

- \(\bar{v}\) = fluid velocity
- \(p\) = fluid pressure
- \(g\) = gravity vector which is defined in relation to vertical elevation
  \(\bar{g} = |\bar{g}|V\) (Elevation) where \(|\bar{g}|\) is the magnitude of gravitational acceleration and (Elevation) is vertical elevation
- \(k\) = permeability of soil
- \(k_r\) = relative permeability (reduction in permeability due to partial saturation)
- \(\mu\) = viscosity of pore fluid
- \(S_w\) = degree of saturation of soil
- \(\varepsilon\) = porosity of soil
- \(\rho\) = fluid density

The fluid velocity, \(\bar{v}\), is the velocity of fluid passing through the cross sectional area for pore fluid, which is a fraction of total area of the porous medium depending on porosity and saturation. The fluid velocity depends not only on the driving forces for flow that are fluid pressure and bouyancy forces, but also on fluid mobility, which is a combination of permeability, \(k\), relative permeability, \(k_r\), and viscosity of fluid, \(\mu\). Permeability is a property of the porous medium that reflects the ease with which fluid flows through the medium when it is completely saturated. Relative permeability is a reduction factor for
permeability when partial saturation occurs in pores of soil. Viscosity affects the ease of flow of pore fluid and is a function of temperature. The driving forces for flow of fluid through pore volume is combination of fluid pressure and density gradient as in the term $\nabla(p-\rho g)$.

Combining Equations (3-3) and (3-4), Equation (3-5) is obtained, if $\bar{Y}$ is neglected. After simplifying Equation (3-5), Equation (3-6) is obtained.

After simplifying Equation (3-5), Equation (3-6) is obtained.

$$\frac{\partial (\varepsilon S_w p)}{\partial t} = \nabla \left[ \rho \varepsilon S_w \left( \frac{k}{\varepsilon S_w \mu} \right) \left( \nabla p - \rho g \right) \right] + \frac{Q_p}{w}$$ (3-5)

$$\frac{\partial (\varepsilon S_w p)}{\partial t} = \nabla \left[ \rho \left( \frac{k}{\mu} \right) \left( \nabla p - \rho g \right) \right] + \frac{Q_p}{w}$$ (3-6)

Since the primary variables in SUTRA are fluid pressure, $p$, and concentration of solute, $C$, each term in Equation (3-6) was expressed in terms of these primary variables $p$ and $C$. The derivation for the term $\frac{\partial (\varepsilon S_w p)}{\partial t}$ (which is the rate of fluid mass in unit pore volume) derived by Voss and Provost, (2010) is described below in series of equations. Equation (3-7) shows the rate of fluid mass in unit volume in term of partial derivatives of primary variables fluid pressure, $p$ and concentration of solute, $C$.

$$\frac{\partial (\varepsilon S_w p)}{\partial t} = \frac{\partial (\varepsilon S_w p)}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial (\varepsilon S_w p)}{\partial C} \frac{\partial C}{\partial t}$$ (3-7)

Degree of saturation, $S_w$ and $\varepsilon$ depend on fluid pressure, $p$ and fluid density $\rho$ depends on concentration of solute, $C$. In SUTRA, fluid density model is a first order Taylor expansion about a base reference density described, as shown in Equation (3-8) (Voss and Provost, 2010).
\[ \rho = \rho(C) \equiv \rho_0 + \frac{\partial \rho}{\partial C} (C - C_0) \]  

(3-8)

where:

\(\rho\) = density of solution

\(C\) = concentration of solute

\(C_0\) = base solute concentration which is typically zero indicating pure water

\(\rho_0\) = base fluid density at \(C = C_0\) which is typically density of pure water

Therefore, Equation (3-7) can be extended as Equation (3-9).

\[
\frac{\partial (\varepsilon S_w \rho)}{\partial t} = \left[ \left( S_w \frac{\partial (\varepsilon \rho)}{\partial \rho} + \varepsilon \rho \frac{\partial (S_w)}{\partial \rho} \right) \frac{\partial \rho}{\partial t} + \varepsilon S_w \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} \right]
\]

(3-9)

The term \(\frac{\partial (\varepsilon \rho)}{\partial \rho}\) can be related to aquifer storativity under fully saturated conditions as defined below in Equation (3-10) by Bear, (1979).

\[
\frac{\partial (\varepsilon \rho)}{\partial \rho} = \rho S_{op}
\]

(3-10)

where:

\(S_{op}\) = specific pressure storativity

\[
S_{op} = \frac{1}{V_t} \frac{\Delta V_w}{\Delta \rho}
\]

(3-11)

\(V_t\) = total volume

\(V_w\) = volume of pore fluid

\(S_{op}\) = specific pressure storativity

The specific pressure storativity, \(S_{op}\) in SUTRA is defined by Voss and Provost, (2010) as “the volume of water released from saturated pore storage due to a unit drop in fluid pressure per total volume”. The specific pressure storativity, \(S_{op}\) is related to respective compressibilities of pore fluid and bulk porous matrix as shown in Equation (3-12). The
details of this derivation is included in SUTRA documentation prepared by Voss and Provost, (2010).

\[ S_{op} = (1-\varepsilon)\alpha + \varepsilon\beta \]  \hspace{1cm} (3-12)

where:

\[ \alpha = \text{porous matrix compressibility is an input parameter in SUTRA. For sand stones, } \alpha \text{ ranges between } 10^{-7} \text{ to } 10^{-9} \text{ Pa}^{-1}. \]

\[ \beta = \text{compressibility of pore fluid is also an input parameter in SUTRA, for water } \beta = 4.471 \times 10^{-10} \text{ Pa}^{-1}. \]

The term \( \frac{\partial (S_w)}{\partial p} \) in Equation (3-9) is incorporated in the unsaturated model of SUTRA, which was defined by van Genuchten, (1980) as was presented in Equation (3-2) where capillary pressure, \( p_c = -p \). In SUTRA, this term appears only when negative pressures are solved by SUTRA in an unsaturated zone.

Combining Equations (3-9) and (3-10), Equation (3-13) was obtained.

\[
\frac{\partial (\varepsilon S_w \rho)}{\partial t} = \left[ \left( S_w \rho S_{op} + \varepsilon \rho \frac{\partial (S_w)}{\partial p} \right) \frac{\partial p}{\partial t} + \varepsilon S_w \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} \right] \]  \hspace{1cm} (3-13)

The fluid mass balance equation in SUTRA was obtained as in Equation (3-14) shown below by combining Equations (3-13) and (3-6).

\[
\left( S_w \rho S_{op} + \varepsilon \rho \frac{\partial S_w}{\partial p} \right) \frac{\partial p}{\partial t} + \varepsilon S_w \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \nabla \left[ \frac{k \rho}{\mu} \nabla (\rho g) \right] = Q_p \]  \hspace{1cm} (3-14)

where:

\[ v = \text{fluid velocity} \]

\[ p = \text{fluid pressure} \]

\[ C = \text{concentration of solute} \]
\( \mathbf{g} \) = gravity vector which is defined in relation to vertical elevation
\( \mathbf{g} = \left| \mathbf{g} \right| \nabla \text{(Elevation)} \) where \( \left| \mathbf{g} \right| \) is the magnitude of gravitational acceleration and (Elevation) is vertical elevation

\( k \) = permeability of soil

\( k_r \) = relative permeability (reduction in permeability due to partial saturation)

\( \mu \) = viscosity of pore fluid

\( S_w \) = degree of saturation of soil

\( \varepsilon \) = porosity of soil

\( \rho \) = fluid density

\( Q_p \) = fluid mass source (including pure water mass plus solute dissolved in source water)

\( S_{op} \) = specific pressure storativity

Since specific pressure storativity \( S_{op} \) concept is for fully saturated soils, it is not exactly valid for unsaturated media, nevertheless the error that it brings into Equation (3-14) is insignificant since \( \frac{\partial S_w}{\partial p} \gg S_{op} \).

Equation (3-14) shows the time-dependent relationship between the mass of pore fluid flowing through unit pore volume as a function of primary variables fluid pressure, \( p \) and concentration of solute, \( C \). Equation (3-14) accounts for the change in degree of saturation as a function of fluid pressure and change in density as a function of concentration of solute. As mentioned before the change in degree of saturation occurs only in capillary zone with negative pore pressure.

In SUTRA-Bubble, which simulates partial saturation created by IPS, partial saturation occurs below the water table in the so called “saturated” zone in SUTRA.
Therefore, a new term representing the IPS defined partial saturation condition was necessary. A total degree of saturation term, $S_w^t$ was defined as shown in Equation (3-15). This total degree of saturation term was defined as the multiplication of the degree of saturation in capillary zone (defined in SUTRA), $S_w$ and the degree of saturation created by IPS, $S_w^b$.

$$S_w^t = S_w^b \times S_w$$  \hspace{1cm} (3-15)

where:

- $S_w^b$ = degree of saturation created by IPS
- $S_w$ = degree of saturation term in SUTRA defined in capillary zone

Equation (3-15) demonstrates that when $S_w^b = 1$ in the capillary zone above the water table $S_w^t = S_w$ as in SUTRA and when $S_w = 1$ which is the case for IPS below the water table, then $S_w^t = S_w^b$.

In SUTRA-Bubble, the degree of saturation created by IPS, $S_w^b$ is related to the amount of gas bubbles as well as the absolute pressure of gas bubbles using Ideal gas law. Also, modifications in the main governing equation for flow, mass balance equation (Equation 3-14) was needed to incorporate formulations of $S_w$, and $S_w^b$ in order to simulate the flow in partially saturated soils created by IPS.

Subsequent sections describe the theoretical formulations of $S_w^b$ using the ideal gas law followed by the theoretical formulations of the modifications in fluid mass-balance equation. Specifically, two constitutive models are described. The first model is for gas generation where the amount of gas bubbles is numerically solved using the reactivity of
the solute. The second model is for relative permeability coefficient, which is determined as a power function of degree of saturation. In addition, details of the fluid density model incorporated in SUTRA-Bubble are included. The chapter finishes with the structure of the modifications in the coding of SUTRA-Bubble.

3.2 Theoretical Formulations in SUTRA-Bubble

In this section, formulation of the degree of saturation as a function of amount of gas bubbles, and gas pressure is presented. This is followed by the formulations of the modifications in the main flow equation (mass-balance equation) of SUTRA incorporating $S_w$ and $S_w^b$.

3.2.1 Degree of Saturation Equation in SUTRA-Bubble

The degree of saturation is the most important parameter to be solved by SUTRA-Bubble. The ideal gas law is used to relate the amount of gas to the volume of the gas, which determines the degree of saturation in a closed controlled volume under certain pressure conditions.

The following assumptions were made in use of the ideal gas law:

- There is no change in porosity of the soil.
- Gas bubbles are formed in the pore space of the sand below the water table. There are no capillary pressures.
- The total volume of the gas bubbles is smaller than the total volume of void space.
- Gas bubbles are suspended in the pore fluid and thus connected to the atmospheric pressure through the pore fluid.
- Surface tension between gas bubbles and the water is small and neglected. Therefore, gas bubble pressure is equal to the positive fluid pressure.
- Gas bubbles are all of the same size and behave identically.
- Gas bubbles are trapped within the pore space of the sand.
- Temperature is constant.

**Formulation of degree of saturation equation**

Equation (3-16) presents the Ideal gas law relating volume of gas to moles of gas and pressure of gas, which is equal to fluid pressure.

\[ p_b V_b = n_b R T \]  

(3-16)

where:
- \( p_b = p^* + p \)
  - \( p_b \) = pressure of gas bubbles
  - \( P^* \) = atmospheric pressure
  - \( p \) = fluid pressure in SUTRA
  - \( V_b \) = volume of gas bubbles
  - \( n_b \) = mole of gas bubbles
  - \( R \) = gas constant
  - \( T \) = constant temperature

Rearrangement of Equation (3-16) to solve for volume gives

\[ V_b = \frac{n_b R T}{p_b} \]  

(3-17)

In order to relate the volume of gas to degree of saturation, both sides of Equation (3-17) were divided by the volume of voids presented by \( V_v \). Equation (3-18) shows the normalized version of Equation (3-17).
\[
\frac{V_b}{V_v} = \frac{n_b}{V_v} \frac{RT}{p_b}
\]  (3-18)

\[
\frac{V_b}{V_v} = \frac{V_v - V_w}{V_v} = 1 - \frac{V_w}{V_v} = 1 - S_w^b
\]  (3-19)

where \( V_w \) is volume of fluid in the pore space and \( S_w^b = \frac{V_w}{V_v} \).

\[
\frac{n_b}{V_v} = \frac{n_b}{V_w} \frac{V_w}{V_v} = n_b S_w^b
\]  (3-20)

where:

\( n_b \) is molar concentration of gas bubbles and \( S_w^b = \frac{V_w}{V_v} \) is the degree of saturation in SUTRA-Bubble.

Substituting Equations (3-19) and (3-20) into Equation (3-18), below Equation (3-21) was obtained.

\[
1 - S_w^b = n_b S_w^b \frac{RT}{p_b}
\]  (3-21)

Rearranging Equation (3-21), the final form of degree of saturation, \( S_w^b \) as a function of absolute pressure of gas, \( p_b \), molar concentration of gas, \( n_b \), gas constant, \( R \), and constant temperature, \( T \) is shown in Equation (3-22).

\[
S_w^b = \frac{p_b}{p_b + n_b RT}
\]  (3-22)
Equation (3-22) shows that the degree of saturation, $S_{w}^{b}$, is equal to 1 when molar concentration of gas, $v_{b}$, is zero, indicating no gas bubble generation. Also, with increasing molar concentration of gas, the degree of saturation decreases, indicating partial saturation. Moreover, the equation indicates that as the absolute pressure of the gas bubbles, $p_{b}$, increases, the degree of saturation increases due to the decrease in volume of gas under larger pressure. This is consistent with ideal gas law.

The next section describes the formulation of the flow equation (fluid mass-balance equation, Equation (3-14)) modified using degree of saturation, $S_{w}^{c}$ and $S_{w}^{b}$.

### 3.2.2 Flow Equation in SUTRA-Bubble

The fluid mass-balance equation in SUTRA, Equation (3-14), was formulated using the degree of saturation, which is related to capillary pressure in unsaturated zone. In SUTRA-Bubble, the mass balance equation was formulated using the total degree of saturation, $S_{w}^{t}$, which is the product of the degree of saturation in capillary zone (defined in SUTRA), $S_{w}$, and the degree of saturation created by IPS, $S_{w}^{b}$, as was shown in Equation (3-15).

**Formulation of fluid mass-balance equation in SUTRA-Bubble**

The fundamental form of the fluid mass-balance equation was presented in Equation (3-6). Equation (3-6) is re-written again using total degree of saturation, $S_{w}^{t}$, instead of $S_{w}$ (degree of saturation in the capillary zone defined in SUTRA) as shown in Equation (3-23) below.
Equations (3-24) and (3-25) show $\frac{\partial (\varepsilon S^i_w \rho)}{\partial t}$ in terms of partial derivatives of primary variables fluid pressure, $p$ and concentration of solute, $C$. 

$$\frac{\partial (\varepsilon S^i_w \rho)}{\partial t} = \varepsilon p \frac{\partial (S^i_w)}{\partial t} + S^i_w \frac{\partial (\varepsilon p)}{\partial t} \tag{3-24}$$

$$\frac{\partial (\varepsilon S^i_w \rho)}{\partial t} = \varepsilon p \frac{\partial (S^i_w)}{\partial t} + S^i_w \left[ \frac{\partial (\varepsilon p)}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial (\varepsilon p)}{\partial C} \frac{\partial C}{\partial t} \right] \tag{3-25}$$

where;

$$\frac{\partial (\varepsilon p)}{\partial p} = \rho S_{\varepsilon p} \quad \text{and} \quad S_{\varepsilon p} = (1-\varepsilon)\alpha + \varepsilon \beta \quad \text{similar to formulations in SUTRA.}$$

Time derivative of total degree of saturation, $\frac{\partial (S^i_w)}{\partial t}$ was formulated in SUTRA-Bubble as follows:

**Time derivative of total degree of saturation**

Equation (3-15) which relates total degree of saturation as multiplication of $S_w$ and $S^i_w$ and Equation (3-22) which relates $S^b_w$ to absolute pressure of gas, $p_b$, molar concentration of gas, $v_b$, gas constant, $R$, and constant temperature, $T$ are shown again below for reference.

$$S^i_w = S^b_w \times S_w$$

and
\[ S_w^b = \frac{p_b}{p_b + v_bRT} \]

Using Equations (3-15) and (3-22), the time derivative of \( S_w^i \) was formulated using the multiplication rule.

\[
\frac{\partial S_w^i}{\partial t} = S_w^i \frac{\partial S_w}{\partial P} \frac{\partial P}{\partial t} + S_w^i (1 - S_w^b) \frac{\partial P}{\partial t} - S_w^i RT \left( S_w^b \right)^2 \frac{\partial v_b}{\partial t} \tag{3-26}
\]

When \( S_w = 1.0 \), Equation (3-26) becomes:

\[
\frac{\partial S_w^i}{\partial t} = S_w^b (1 - S_w^b) \frac{\partial P}{\partial t} - RT \left( S_w^b \right)^2 \frac{\partial v_b}{\partial t} \tag{3-27}
\]

Substituting the derivative of \( S_w^i \) shown in Equation (3-27) into Equation (3-25), the following is obtained. Equation (3-28) shows the change in fluid mass per unit volume with time, \( \frac{\partial (\varepsilon S_w^i \rho)}{\partial t} \) in SUTRA-Bubble for the simulation of partial saturation created by IPS when \( S_w = 1.0 \) and thus \( S_w^i = S_w^b \)

\[
\frac{\partial (\varepsilon S_w^i \rho)}{\partial t} = \varepsilon \rho \left[ S_w^b (1 - S_w^b) \frac{\partial P}{\partial t} - RT \left( S_w^b \right)^2 \frac{\partial v_b}{\partial t} \right] + S_w^b \left[ \frac{\partial (\varepsilon \rho)}{\partial P} \frac{\partial P}{\partial t} + \frac{\partial (\varepsilon \rho)}{\partial C} \frac{\partial C}{\partial t} \right] \tag{3-28}
\]

Finally, the modified mass-balance equation in SUTRA-Bubble was obtained by substituting Equation (3-28) in Equation (3-23).
The new terms in the mass-balance equation in SUTRA-Bubble are highlighted in Equation (3-29). The rate of change in molar concentration of gas bubbles appears in the modified mass-balance equation (Equation 3-29). The contribution of molar concentration of gas bubbles to the outflow of the pore fluid from a unit volume is represented by the term $RT\varepsilon\rho\left(\frac{S_w^b}{P_b}\right)^2 \overcox{\partial u_b}{\partial t}$. The change in volume of gas bubble due to change in fluid pressure is shown by the term $\varepsilon\rho\left(1-\frac{S_w^b}{P_b}\right) \overcox{\partial P}{\partial t}$. This term represents the change in effective storativity because of the existence of gas bubbles which makes the pore fluid more compressible.

The following section describes the constitutive models incorporated in SUTRA-Bubble.

### 3.3 Constitutive Models in SUTRA-Bubble

Two constitutive models were developed and incorporated in SUTRA-Bubble, namely: for gas generation and for relative permeability.

#### 3.3.1 Constitutive Model for Gas Generation in Soil

In SUTRA-Bubble, gas generation is related to the chemical decomposition of the solute in the pore fluid. As the solute decomposes, gas bubbles are generated over time with certain mole fractions. For example, $m$ moles of solute generates $n$ moles of gas.
bubbles at the end of reaction, under ideal conditions (100% efficiency). The ratio of \( \frac{n}{m} \) is referred to as \( \delta \), the stoichiometric coefficient for gas generation.

By tracing the change in the concentration of solute, the increase in the moles of gas can be determined using the stoichiometric coefficient, \( \delta \). Typically, a chemical decomposition follows an exponential rate expression. A first order decay which results in exponential decomposition of the concentration of solute was already programmed in SUTRA. Figure 3-2 shows the proposed constitutive model for production of gas as a result of the chemical decomposition of solute.

![Schematic for the constitutive model for gas generation in SUTRA-Bubble](image)

The following assumptions were made to relate the rate of decrease in concentration of solute to the moles of gas generated:

- The rate of production of gas is proportional to the rate of decomposition of solute.
- The stoichiometric coefficient for gas generation \( \delta \) is constant at any time of the chemical reaction.
- The pore fluid is water.
Rate of Decomposition of Solute

The relationship for the decomposition concentration of solute is shown below in Equation (3-30).

\[ C(t) = (C_0) \exp(-rt) \quad (3-30) \]

where:
- \( C(t) \) = concentration of solute at time \( t \)
- \( C_0 \) = initial concentration of solute
- \( r \) = rate parameter

Differentiating Equation (3-30), the rate of concentration of solute is given by Equation (3-31).

\[ \frac{\Delta C}{\Delta t} = -r(C_0)(\exp(-rt)) = -rC \quad (3-31) \]

SUTRA incorporates the exponential decomposition of concentration of solute through Equation (3-32).

\[ \Gamma_w = \gamma_1^w C \quad (3-32) \]

where:
- \( \Gamma_w \) = rate of solute mass per unit fluid mass = \( \frac{\Delta C}{\Delta t} \) in Equation (3-30)
- \( \gamma_1^w \) = SUTRA rate parameter

In SUTRA-Bubble, the rate parameter \( \gamma_1^w \) is equal to the negative of the rate parameter, \( r \),

\[ \gamma_1^w = -r \], indicating decomposition. The rate parameter \( \gamma_1^w \) is an input of SUTRA-Bubble simulation.
Rate of Production of Gas Bubbles:

The rate of production of gas bubbles is related to the rate of decomposition of solute is presented in Equation (3-33).

\[
\frac{\Delta u_b}{\Delta t} = F \cdot \left( -\frac{\Delta C}{\Delta t} \right)
\]  

(3-33)

where:

\( u_b \) = molar concentration of gas bubbles  
\( C \) = concentration of solute  
\( F \) = unit conversion parameter

In order to relate the two rates, the units for both sides of the equation should be consistent. Therefore, the unit conversion parameter should be determined to relate the concentration of solute to the molar concentration of gas bubbles. The units for concentration of solute and molar concentration of gas bubbles defined in SUTRA-Bubble are shown below.

Concentration of solute, \( C \left( \frac{kg}{kg} \right) \)

and:

Molar concentration of gas bubbles, \( u_b \left( \frac{mole}{m^3} \right) \)

\[
u_b \left( \frac{mole}{m^3 \text{ of fluid}} \right) = C \left( \frac{kg \text{ of solute}}{kg \text{ of fluid}} \right) \times \rho \left( \frac{kg \text{ of fluid}}{m \text{ of fluid}} \right) \times \frac{1}{MW_{\text{solute}}} \left( \frac{mole \text{ of solute}}{kg \text{ of solute}} \right) \times \delta \left( \frac{mole \text{ of gas}}{mole \text{ of solute}} \right)
\]

Equations (3-34) relates to \( C \) and the defined \( F \) parameter is presented as in Equation (3-35).

\[
u_b = \frac{\rho \delta}{MW_{\text{solute}}} \cdot C
\]  

(3-34)
\[
F = \frac{\rho \delta}{MW_{\text{solute}}} \tag{3-35}
\]

where:
\[
\delta = \text{stoichiometric coefficient for chemical reaction}
\]
\[
\rho = \text{density of solution}
\]
\[
MW_{\text{solute}} = \text{molecular weight of the chemical}
\]

Combining Equations (3-33) and (3-35), Equation (3-36) relating the rate of gas bubble production to the rate of decomposition of the solute is derived.

\[
\frac{\Delta v_b}{\Delta t} = \left( \rho \frac{\delta}{MW_{\text{solute}}} \right) \left( -\frac{\Delta C}{\Delta t} \right) \tag{3-36}
\]

where:
\[
\frac{\Delta C}{\Delta t} = -rC \text{ as was shown in Equation (3-31)}.
\]

Combining Equations (3-31) and (3-36), Equation (3-37) is obtained representing rate of production of gas bubbles.

\[
\frac{\Delta v_b}{\Delta t} = \left( \rho \frac{\delta}{MW_{\text{solute}}} \right) \times (rC) \tag{3-37}
\]

It is noted that the rate parameter, \( r \) for molar concentration of gas in Equation (3-37) is positive indicating the production of gas.

The molar concentration of gas bubbles, \( v_b \) is solved numerically with an initial value of zero, \( v_{b(0)} = 0 \) at the beginning of the reaction. Subsequent value of \( v_{b(i+1)} \) can be obtained from Equation (3-38).

\[
v_{b(i+1)} = v_{b(i)} + \Delta v_b \tag{3-38}
\]
Substituting for $\frac{\Delta v_b}{\Delta t}$ from Equation (3-37) results in Equation (3-39) which gives molar concentration of gas bubbles at any time, $t$.

$$v_{b(i+1)} = v_{b(i)} + \left[ \frac{\delta \rho}{MW_{\text{solute}}} r C \right] \Delta t \quad (3-39)$$

where:

- $v_b$ = molar concentration of gas bubbles
- $C$ = concentration of solute
- $\delta$ = stoichiometric coefficient for chemical reaction
- $\rho$ = density of solution
- $MW_{\text{solute}}$ = molecular weight of the chemical
- $r$ = rate parameter

The application of IPS uses sodium percarbonate solution to generate gas bubbles in the pores of sand. Typically, the solution is prepared with a specific concentration of the sodium percarbonate powder, referred to $C_{\text{SPC}}$. The solute that generates the gas bubbles is hydrogen peroxide ($H_2O_2$), as shown in the following chemical reaction.

$$\begin{align*}
\text{Na}_2\text{CO}_3.1.5\text{H}_2\text{O}_2 \quad \text{in water} & \rightarrow 2\text{Na}^{+1} + \text{CO}_3^{2-} + 1.5\text{H}_2\text{O}_2 \\
1.5\text{H}_2\text{O}_2 \quad \text{in water} & \rightarrow 1.5\text{H}_2\text{O} + 0.75\text{O}_2
\end{align*}$$

(at the end of reaction)

(ideal conditions - 100% efficiency)

Therefore, the initial concentration of solute, $C_0$, used in SUTRA-Bubble is the concentration of hydrogen peroxide, $C_{H_2O_2}$. The initial concentration of hydrogen peroxide can be related to the concentration of the sodium percarbonate from the chemical reaction by:

$$C_{H_2O_2} = 1.5 \frac{C_{\text{SPC}}}{MW_{\text{SPC}}} MW_{H_2O_2} \quad (3-40)$$
where:

\[ C_{H_2O_2} = \text{mass concentration of hydrogen peroxide} \]

\[ C_{SPC} = \text{mass concentration of sodium percarbonate} \]

\[ MW_{H_2O_2} = \text{molecular weight of hydrogen peroxide} = 0.034 \text{ kg} \]

\[ MW_{SPC} = \text{molecular weight of sodium percarbonate} = 0.157 \text{ kg} \]

It is noted that the instantaneous dissociation of sodium percarbonate into sodium and carbonate ions and hydrogen peroxide is assumed to be completed before hydrogen peroxide starts generating gas bubbles. In Equation (3-40), the chemical reaction for gas generation was then assumed to be under ideal conditions where the efficiency of production of gas, \( E_f \) is 100%. However, this assumption is unrealistic, and the actual yield of gas might be lower. Introducing the efficiency factor, \( E_f \) in Equation (3-40), and equating concentration of hydrogen peroxide to concentration of solute, \( C \), used in SUTRA-Bubble, results:

\[
C = C_{H_2O_2} = E_f \times \left( 1.5 \frac{C_{SPC}}{MW_{SPC}} \frac{MW_{H_2O_2}}{MW_{SPC}} \right)
\]

where:

\[ C = \text{concentration of solute in SUTRA-Bubble (} C_{H_2O_2} \text{)} \]

\[ E_f = \text{efficiency of chemical reaction} \]

The initial concentration of solute, \( C_0 \), is an input parameter to SUTRA-Bubble. In the case of using sodium percarbonate for IPS, Equation (3-41) is used to compute this input for a given \( C_{SPC} \) and \( E_f \).
3.3.2 Constitutive Model for Relative Permeability of Soil

SUTRA allows including a user defined function for relative permeability of a soil as a function of either saturation or capillary pressure. Relative permeability of a soil is a factor that accounts for the reduction in permeability due to partial saturation. In SUTRA-Bubble, the constitutive model to solve for relative permeability as a function of degree of saturation was adopted.

Relative permeability is related to degree of saturation as shown in Figure 3-3.

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

- \( k_{PS} \) - permeability for partially saturated specimen
- \( k_{FS} \) - permeability for fully saturated specimen

Figure 3-3 Relative permeability model in SUTRA-Bubble

In the literature on unsaturated soils, there are a number of empirical relationships for relative permeability published by many researchers (Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980; Bicalho et al. 2000). The relationship suggested by Brooks and Corey (1964) is shown below in Equation (3-42).

\[ k_r = (S_e)^n \]  \hspace{1cm} (3-42)

where \( S_e = \frac{(S_w - S_r)}{(1 - S_r)} \)
Sr is the residual saturation. Sr is assumed to be very small then \( S_e = S_w^i \). \( S_w^i \) is the total saturation defined in SUTRA-Bubble. Also, n is a constant which depends on the soil type. For uniform sands n was determined to be 3 (Irmay, 1954). This was confirmed by Bear (1979) from experiments on soils of uniform grain size agreed with this relationship of 
\[
k_r = \left( \frac{S_w}{S_w^i} \right)^n.
\]

As mentioned in Chapter 2, the partially saturated soil conditions in these studies were in the capillary zone above the water table where the pores pressure was equal to the matric suction. Therefore, relative permeability in these types of partially saturated soils was related to the partial saturation, which was due to matric suction. For degree of saturation greater than 80%, it was suggested that the matric suction can be neglected (Bishop and Eldin, 1950). In this research on IPS, the gas bubbles are created within the saturated soil below the water table (no matric suction), and degree of saturation can be lower than 80%. Eseller-Bayat et al. (2013) reported that the degree of saturation of partially saturated specimens prepared by IPS were as low as 40%.

Considering the differences between partial saturation by IPS and partial saturation as considered by Brooks and Corey, (1964 based on capillarity), in this research the exponent n was estimated by performing experiments with partially saturated specimens prepared by ASTM graded Ottawa sand and sodium percarbonate as a gas bubble source. The results from laboratory experiments, which confirm the validity of the general form of the equation for \( k_r \), are presented in Chapter 4.3.
3.4 Fluid Density Model in SUTRA-Bubble

The density difference between the fluid transported and the ambient water will affect flow. SUTRA includes this effect using a density model. The model is a first order Taylor expansion about a base reference density as was described by Equation (3-8). As in SUTRA, in SUTRA-Bubble, base density ($\rho_0$) was assumed to be that of pure water with base concentration ($C_0$) of 0. In Equation (3-8), the density of the ambient pore fluid is adjusted as the concentration changes due to arrival of solution.

In the SUTRA-Bubble simulations, it is noted that the concentration of solute, $C$, is that of hydrogen peroxide which is the source of oxygen gas. SUTRA-Bubble does not track separate concentrations of sodium and carbonate ions and hydrogen peroxide. The transport of the ions are not significantly important since they do not contribute to the gas bubble generation. Their effect is only on the density of the solution. The rate factor $\frac{\partial \rho}{\partial C}$ determines the density of solution at a certain concentration of sodium percarbonate. In an IPS application, variability in the density of the fluid within a sand medium affects the flow. In order to determine the rate factor, $\frac{\partial \rho}{\partial C}$, the total density of sodium percarbonate solution was related to the concentration of hydrogen peroxide. By means of this, the equivalent $\frac{\partial \rho}{\partial C}$ term indirectly included the density effect of the sodium and carbonate ions. Derivation of $\frac{\partial \rho}{\partial C}$ is presented below. Equation (3-8) is presented again below for reference.
\[ \rho = \rho(C) = \rho_o + \frac{\partial \rho}{\partial C}(C-C_o) \]

where:

\( \rho_o \) is the density of pure water (base fluid) and \( \rho_o = \rho_{water} \) with base concentration,

\[ C_o = 0.0 \left( \frac{kg}{kg} \right) \]

Equation (3-8) then becomes Equation (3-43) shown below.

\[ \rho(C) = \rho_{water} + \frac{\partial \rho}{\partial C}(C-0) \quad (3-43) \]

where:

\( \rho(C) \) is the density of sodium percarbonate solution with concentration of \( C_{SPC} \).

The density of solution, \( \rho(C) \), is related to its molecular weight \( MW_{SPC} \) and the volume \( V_{solution} \) of sodium percarbonate solution as shown in Equation (3-44) below.

\[ \rho(C) = \frac{M_{SPC} + M_{water}}{V_{solution}} \quad (3-44) \]

Since volume share of sodium percarbonate powder in the solution is negligible, it can be assumed that \( V_{solution} = V_{water} \). Then, Equation (3-44) becomes Equation (3-45).

\[ \rho(C) = \frac{M_{water} + M_{SPC}}{V_{water}} = \frac{M_{water}}{V_{water}} + \frac{M_{SPC}}{V_{water}} = \frac{M_{water}}{V_{water}} + \frac{M_{SPC}}{M_{water}} \cdot \frac{M_{water}}{V_{water}} \quad (3-45) \]

Combining Equations (3-43) and (3-45), Equation (3-46) was obtained as shown below.
\[
\rho_{\text{water}} + \left( C_{\text{SPC}}\rho_{\text{water}} \right) = \rho_{\text{water}} + \frac{\partial \rho}{\partial C}(C-0) \quad (3-46)
\]

where:

\[C_0 = C_{\text{H}_2\text{O}_2} = E_f \times \left( 1.5 \frac{C_{\text{SPC}}}{\text{MW}_{\text{SPC}}} \cdot \text{MW}_{\text{H}_2\text{O}_2} \right) \] as was presented in Equation (3-41).

\[C_0 = \text{initial concentration of solute in SUTRA-Bubble (concentration of hydrogen peroxide)}\]

\[C_{\text{H}_2\text{O}_2} = \text{mass concentration of hydrogen peroxide}\]

\[E_f = \text{efficiency of chemical reaction}\]

\[C_{\text{SPC}} = \text{mass concentration of sodium percarbonate}\]

\[\text{MW}_{\text{H}_2\text{O}_2} = \text{molecular weight of hydrogen peroxide}\]

\[\text{MW}_{\text{SPC}} = \text{molecular weight of sodium percarbonate}\]

Substitution of Equation (3-41) in Equation (3-46) yields into Equation (3-47).

\[
\rho_{\text{water}} + \left( C_{\text{SPC}}\rho_{\text{water}} \right) = \rho_{\text{water}} + \frac{\partial \rho}{\partial C} \left( E_f \times 1.5 \frac{C_{\text{SPC}}}{\text{MW}_{\text{SPC}}} \cdot \text{MW}_{\text{H}_2\text{O}_2} \right) \quad (3-47)
\]

Rearranging Equation (3-47), rate term \[\frac{\partial \rho}{\partial C}\] can be related to efficiency, \(E_f\), molecular weights of sodium percarbonate, \(\text{MW}_{\text{SPC}}\), hydrogen peroxide, \(\text{MW}_{\text{H}_2\text{O}_2}\) and density of pure water, \(\rho_{\text{water}}\) as described in Equation (3-48).

\[
\frac{\partial \rho}{\partial C} = E_f \frac{\rho_{\text{water}} \cdot \text{MW}_{\text{SPC}}}{1.5 \cdot \text{MW}_{\text{H}_2\text{O}_2}} \quad (3-48)
\]

It is noted that \[\frac{\partial \rho}{\partial C}\] term does not depend on the value of the concentration. It depends on the efficiency, \(E_f\), the value determined from laboratory experiments.
In SUTRA-Bubble the concentration of solute is that of hydrogen peroxide, which decays as it reacts with water, generating oxygen gas. Therefore, as hydrogen peroxide decays, SUTRA-Bubble will reduce the density of the solute and hence the solution. In reality, density of sodium percarbonate solution is determined by the weight of sodium and carbonate ions, as well as hydrogen peroxide. Since the sodium and carbonate ions do not decay, the density of the sodium percarbonate solution should decrease to some extent as hydrogen peroxide reacts depending on its mass fraction in sodium percarbonate. Ideally the effect of sodium and carbonate ions on the density of sodium percarbonate solution should not be ignored. Otherwise it leads to an underestimation of the fluid density effect on flow, during the period of gas generation Figure 3-4 shows a schematic describing the fluid density in SUTRA-Bubble during the course of the simulation, starting and ending of injection of fluid and subsequent bubble generation (Case A).

![Schematic showing the fluid density change over the course of the simulation](image)

**Figure 3-4** Schematic showing the fluid density change over the course of the simulation

During injection of solution of sodium percarbonate, the fluid density, $\rho$ increases within the zone of influence of the injection as the concentration of solution at that point
increases till it reaches the maximum density $\rho \left( C_{\text{spec}} \right)$ of the design concentration of the solution. After injection ends, when there is no more supply of sodium percarbonate solution, density should reduce only slightly because of decay of hydrogen peroxide. However, because SUTRA-Bubble tracks density change with the decaying concentration of hydrogen peroxide (Case A) it overestimates the density decrease and underestimates the flow effect of density. The trend depicted as Case B in the Figure 3-4 shows the upper limit for the fluid density effect, where the fluid density is not affected by the decay of hydrogen peroxide and by diffusion of the ions. In reality, even though the sodium and carbonate ions do not decay over time, they are still transported through diffusion with the concentration gradient. Therefore, Case B is considered as extreme case where the effect of fluid density is overestimated. The rate of decrease in density after the end of injection should be somewhere between Case A and Case B.

The underestimation of the effect of density by SUTRA-Bubble was evaluated. It is noted that even in the overestimated case (Case B), the maximum increase in density of the fluid is 1% when the concentration of sodium percarbonate is 1%. Typical sodium percarbonate concentrations used in IPS are less than 1% by weight. Since the typical increase in fluid density is quite small, it can be assumed that its effect on flow and subsequent zone of partial saturation is also small.

In order to support this, the typical pressure gradient during injection of solution and the gradient due to fluid density beyond injection were compared. Selected results of SUTRA-Bubble simulations made for laboratory experiments are used to quantify the effect of the hydraulic gradient and the fluid density on flow. The results represent typical hydraulic gradients that may be used in field implementation of IPS. The density gradient
compared to the injection pressure gradients was calculated at three critical locations (Points A, B, C) as shown in Figure 3-5. The figure shows a typical concentration output from a SUTRA-Bubble simulation showing the size of the zone of influence of the injection. Point A is very close to the injection tip, where the highest pressures were computed. Point B is selected at a location which is slightly inside the zone of influence, and Point C is slightly outside the zone of influence.

![Figure 3-5 Concentration output of SUTRA-Bubble showing the selected locations of Points A, B, and C](image)

The driving force ratio concept proposed by Davies (1987) was used to determine the effect of density relative to the injection pressure of flow. Equation (3-49) shows the proposed ratio:

\[
DFR = \frac{\Delta \rho |\nabla E|}{\rho_f |\nabla H_f|} \tag{3-49}
\]

where:
- \(DFR\) = driving-force ratio (dimensionless)
- \(|\nabla E|\) = magnitude of the gradient of elevation (dimensionless)
\[ |\nabla H_f| \] = magnitude of the equivalent water head gradient (dimensionless)

\[ \Delta \rho \] = difference between actual fluid density and clean water density

\[ \rho_f \] = density of water

Equation (3-49) was applied at points A, B, and C shown in Figure 3-5

Figure 3-5. Since the pressure gradient from A to B is quite large, the driving force ratio is expected to be low. The pressure gradient from B to C is very low, because the points are away from the injection tip, the driving force ration is expected to be high. The calculation of the driving force ratio for the two regions A to B and B to C are as follows:

Since vertical flow was assumed, \( \nabla E = 1.0 \) in the equation.

\[ |\nabla H_f| \] in Equation (3-49) for both regions A to B and B to C is calculated by getting total head for each point.

\[
H_f = \frac{p}{\rho_w |g|} + E
\]

(3-50)

where:

\( H_f \) = total head of water

\( \rho_w \) = density of water

\( E \) = elevation head

\( p \) = fluid pressure

The results of calculations of total heads at points A, B, and C using Equation (3-50) follow:

**H<sub>f</sub> at A:**

\[
H_f @ A = \frac{3810}{1000 (9.81)} + (-0.255) = 0.134 \text{ m}
\]

\( p = 3810 \) Pa (during injection)

\( E = -0.255 \) m

\( \rho_f = 1000 \) kg/m\(^3\)

\( |g| = 9.81 \) m/s\(^2\)
Using the calculated values of $H_f$, the driving force ratios (DFR) (Equation 3-49) were calculated for the regions of A to B and B to C as follows:

**DFR from A to B**

$$|\nabla H_f|_{\text{from A-B}} = \frac{0.134 - 0.0427}{-0.255 - (-0.47)} = 0.425$$

$$\text{DFR} = \frac{10}{1000 (0.425)} = 0.024$$

**DFR from B to C**

$$|\nabla H_f|_{\text{from B-C}} = \frac{0.0427 - 0.0421}{-0.47 - (-0.49)} = 0.03$$

$$\text{DFR} = \frac{10}{1000 (0.03)} = 0.33$$
DFR in the region of B to C (0.33) is larger than that of A to B (0.024); indicating that the density effect on flow in the region of B to C is higher due to smaller pressure gradient. However, this value of DFR=0.33 is still lower than the threshold value of DFR=0.5 published by Davies, (1987). The threshold value is the limit above which density effects on the flow can be significant. Moreover, the size of the region B to C compared to A to B is a lot smaller. Based on these discussions, it can be concluded that the effect of gradient due to fluid density compared to the gradient due to pressure on the zone of influence is not significant during the injection period.

The potential slight effect of density on flow past the time of the end of injection on the size of partial saturation zone was estimated analytically using 1D flow approach. For the case of B (Figure 3-4) vertical travel distance of the fluid under the maximum fluid density was estimated using 1D Darcy’s velocity equation proposed by Davies (1987), as in Equation (3-51).

\[
\bar{v} = -K \left[ \nabla H_f + \frac{\Delta \rho}{\rho_w} \nabla E \right]
\]

(3-51)

where:

\(\bar{v}\) = Darcy’s velocity

\(K\) = permeability

\(\nabla H_f\) = gradient of water head

\(\nabla E\) = gradient of elevation

\(\Delta \rho\) = difference between actual fluid density and clean water density

\(\rho_w\) = density of water

The following conservative assumptions were made in the calculations:

- 1D vertical flow (\(\nabla E=1\))
• Density induced flow that may impact the zone of partial saturation is considered for a period of 2 hours during which hydrogen peroxide completes its decomposition.

• The difference between the density of solution and density of clean water \( \Delta \rho \) remains at its maximum (Case B in Figure 3-4).

• Reduction in permeability due to partial saturation was ignored which accentuated the density-driven flow.

After termination of injection, \( \nabla H_f = 0 \), and considering 1D vertical flow \( E = 1 \).

Substituting these values in Equation (3-51) yields Equation (3-52).

\[
\frac{-v}{v} = -K\left[\frac{10}{1000}\right] = -0.01 K \quad (3-52)
\]

where:

\[
\rho_f = 1000 \left(\frac{kg}{m^3}\right) \quad \text{and for } CSPC = 1\% = 0.01 \left(\frac{kg}{kg}\right) \quad \text{leading to } \Delta \rho = 10 \left(\frac{kg}{m^3}\right)
\]

It is noted that the Darcy’s velocity due to only density gradient depends on the permeability of the sand.

The permeability values obtained for the sand specimens tested in this research were: 1) \( 5 \times 10^{-4} \) m/s for sand specimen in the Laminar Box tests presented in Chapter 6, and 2) \( 1.5 \times 10^{-3} \) m/s from controlled laboratory experiments (glass tank experiments) presented in Chapter 5. These values for permeability were in the range of typical field values \( 10^{-3} \) to \( 10^{-5} \) m/s) for sands. It is noted that the permeability value obtained in the laboratory experiments is on the high end of the typical range for sands because the specimen prepared was very loose. For this reason, the effect of density using large permeability value is overestimated.
Using Equation (3-52) Darcy’s velocity and vertical fluid travel distance, $d_w$ for 2 hrs are calculated as follow:

**For $K = 5 \times 10^{-4} \text{ m/s}$ in Laminar Box test:**

$$\bar{v} = -0.01K = 5 \times 10^{-6} \text{ m/s}$$

$$d_w = 5 \times 10^{-6} \times (2 \times 60 \times 60) = 3.6 \text{ cm}$$

**For $K = 1.5 \times 10^{-3} \text{ m/s}$ in glass tank experiments:**

$$\bar{v} = -0.01K = 1.5 \times 10^{-5} \text{ m/s}$$

$$d_w = 1.5 \times 10^{-5} \times (2 \times 60 \times 60) = 10.8 \text{ cm}$$

Under most conservative assumptions, which would lead to overestimation of flow due to density, the vertical expansion of zone of partial saturation may range between 4 and 11 cm.

The vertical distance for the predicted partial saturation zone by SUTRA-Bubble with underestimated density effect was approximately 35 cm in Laminar Box experiments and approximately 30 cm in glass tank experiments. In the case of the glass tank, the vertical flow was constrained by the closeness of the bottom of the tank to the injection head. The grossly overestimated effect of density on flow, hence on the zone of partial saturation, (4 to 11 cm) compared with the 30 to 35 cm zone predicted by SUTRA-Bubble is modest. From the practical point of view, field implementation of IPS will involve variability in concentration, pressure, and permeability. SUTRA-Bubble simulations of the IPS field process will also have a range of predictions. The under-predicting the zone of partial saturation by a few centimeters due to underestimation of density effect will be inconsequential and conservative.
3.5 Modifications of SUTRA Code for SUTRA-Bubble

The SUTRA source code developed by the USGS was modified using the formulations derived in Sections 3.2 and 3.3. This section gives the details of the modifications and additions in the source code of SUTRA made to create SUTRA-Bubble.

The main logic flow of SUTRA program (Figure 5.4 in SUTRA documentation by Voss and Provost, 2010) is presented again in Figure 3-6. The main program called SUTRA_MAIN reads input data to compute the dimensions of the various arrays used by SUTRA, allocates memory for various arrays in SUTRA, starts and stops the simulation. The main control routine, called SUTRA, calls most of the remaining subroutines in sequence in order to initialize the parameters and do calculations for each time step and do iterations (Figure 3-6). The description of each subroutine under the main routine SUTRA is described in the SUTRA documentation (Voss and Provost, 2010). In this section, only the subroutines that needed to be modified are described.

The main logic flow of SUTRA was retained to run SUTRA-Bubble simulations. SUTRA has a subroutine called UNSAT for relating degree of saturation to negative pressure. Since for IPS applications a new degree of saturation was defined, \( S^b_w \), use of UNSAT was no longer sufficient. A new subroutine called BUBSAT was created to solve for \( S^b_w \). SUTRA was prepared such that the UNSAT subroutine is called only if negative pore pressures are solved.
Therefore, the UNSAT subroutine was deactivated and instead BUBSAT was used. The degree of saturation term in the main program SUTRA was changed to a total saturation term, \( S_w^t \), introduced in Equation (3-15) in Section 3.1. The total saturation is

\[ S_w^t = S_w^b \times S_w \]

where:
- \( S_w^b \) = degree of saturation created by IPS in BUBSAT subroutine
- \( S_w \) = degree of saturation in capillary zone in UNSAT subroutine

When \( S_w^b = 1 \) which is the case in the capillary zone above the water table \( S_w^t = S_w \)

When \( S_w = 1 \) which is the case for Induced Partial Saturation (IPS) below the water table \( S_w^t = S_w^b \)

In subroutine BUBSAT, the degree of saturation, \( S_w^b \), and relative permeability, \( k_r \), are calculated. The degree of saturation \( S_w^b \) was defined by Equation (3-22) and the relative permeability as a function of \( S_w^b \) was defined by Equation (3-42).

To solve for \( S_w^b \), the molar concentration of gas bubbles, \( \nu_b \), was required to be defined and initialized as an array in the main control routine SUTRA. The value of \( \nu_b \) was then solved for numerically in the main control routine SUTRA and carried to the subroutine BUBSAT for every time step. The numerical relationship to solve for \( \nu_b \) is shown in Equation (3-39).
In addition to being called in the main control routine SUTRA, the subroutine BUBSAT is called in some of the subroutines as shown in Figure 3-6. The subroutines that call BUBSAT are:

- Subroutine INDAT2, where initial conditions are read.
- Subroutines BASIS2 and BASIS3, where calculations of finite element approximations are made in 2-D and 3-D, respectively.
- Subroutine NODAL, where all calculations of the governing equations both for flow and transport for each node of a mesh are done. Modifications required in the flow equation (Equation (3.13)) were done in this subroutine.
- Subroutine BUDGET, where fluid and solute mass entering and exiting the simulated region are calculated.

Finally, all the constants that are included in the equation for degree of saturation, $S_n^k$, as well as the numerical relationship for molar concentration of gas bubbles are included upfront in the main program SUTRA MAIN. The constants are in units of kilograms for mass, meters for length, seconds for time, and kelvin for temperature. The values of the constant parameters used in the code are listed in Table 3-1.
Figure 3-6 BUBSAT subroutine inserted in the main logic of SUTRA
Table 3-1 Constant values used in SUTRA-Bubble source code

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P^*$ = atmospheric pressure</td>
<td>101325.01 Pa</td>
</tr>
<tr>
<td>$R$ = gas constant</td>
<td>8.3144621 (m$^3$.Pa)/°K.mol</td>
</tr>
<tr>
<td>$T$ = temperature</td>
<td>293 °K</td>
</tr>
<tr>
<td>MW$_{H_2O_2}$ = molecular weight of hydrogen peroxide</td>
<td>0.034 kg</td>
</tr>
<tr>
<td>$\delta$ = stoichiometric coefficient</td>
<td>0.5</td>
</tr>
<tr>
<td>$n$ = saturation exponent in relative permeability relation</td>
<td>2</td>
</tr>
</tbody>
</table>

The code was compiled with the constants dedicated to the chemical reaction of hydrogen peroxide as shown in Table 3-1.

Recompilation of the code is required if

- different units are used to prepare the input files
- a different chemical reaction is modeled, requiring the molecular weight and stoichiometric parameter to change
- a different parameter $n$ is used in the relative permeability equation

The source code of SUTRA is in the Fortran programming language. In this research, the code was edited with Microsoft Visual Studio and compiled with the Intel Visual Fortran Compiler.
Chapter 4

Determination of Parameters for Constitutive Models in
SUTRA-Bubble

4.1 Introduction

This chapter describes laboratory experiments that were conducted in order to
determine the parameters used in the constitutive models of SUTRA-Bubble. As presented
in the previous chapter, there are two new constitutive models in SUTRA-Bubble. The
first model is for gas generation in soils through reactivity of a chemical source. The
second model is for relative permeability to determine the change in soil permeability as a
function of change in degree of saturation in soils.

Equation 3-18, which is duplicated here in Equation (4-1), describes the constitutive
model for gas generation.

\[ u_{b_{i+1}} = u_{b_{i}} + \left[ \frac{\delta \rho}{MW_{\text{solute}}} r C \right] \Delta t \]  

(4-1)
in which \( r \) is the rate parameter that defines the decomposition of the chemical with a
concentration of solute \( C \) as in Equation (4-2).

\[ C(t) = (C_0)e^{(-\pi)} \]  

(4-2)

The rate parameter, \( r \) is an important input in SUTRA-Bubble because it describes
the rate of reaction leading to gas generation and partial saturation of sand. The rate
parameter is sensitive to the environment in which the chemical reaction happens such as
the ion content of the pore water, the type of soil, and the concentration of solute. Therefore, for each specific application of SUTRA-Bubble, an appropriate rate parameter for the chemical reaction should be determined. This chapter will present the experimental estimation of the rate parameter of sodium percarbonate, the value of the rate parameter estimated that was later used to validate SUTRA-Bubble (Chapter 5).

In addition to defining the rate of gas generation, the efficiency of the reaction in generating gas needs to be determined. The efficiency coefficient, $E_f$, for the chemical reaction leading to gas bubbles is also presented in this chapter.

The second constitutive model, the model for relative permeability, was described in Equation (3-42), which is duplicated below in Equation (4-3) for reference.

$$k_r = \frac{k_{Ps}}{k_{FS}} = (S_w^l)^n$$

where:
- $k_{Ps}$ = permeability for partially saturated soil
- $k_{FS}$ = permeability for fully saturated soil
- $S$ = degree of saturation
- $n$ = constant exponent for degree of saturation

In order to determine the parameters for the two constitutive models in SUTRA-Bubble, small scale laboratory experiments were conducted in which the rate of gas generation by sodium percarbonate in the pores of sand specimens was investigated. In addition, constant head permeability tests on partially saturated sands were conducted to determine the relative permeability in the sand tested as a function of degree of saturation.
In all laboratory experiments presented in this dissertation, including constant head permeability for relative permeability measurement, batch experiments for rate of gas generation, and flow experiments to validate SUTRA-Bubble (Chapter 5), ASTM graded Ottawa sand and the chemical called sodium percarbonate were used in order to prepare partially saturated sand specimens.

Ottawa sand (ASTM C778) is a relatively fine silica sand with round and uniformly shaped particles leading to loose sand specimens susceptible to liquefaction. Figure 4-1 shows the grain size distribution curve of the Ottawa sand.

![Ottawa Sand Gradation Curve](image)

Figure 4-1 (a) Picture of ASTM graded C778 sand bag (b) Gradation curve for ASTM C778 Ottawa sand (Eseller-Bayat, 2009)

In this research, sodium percarbonate was used to generate gas bubbles. Sodium percarbonate, Provox ® C, was purchased from the OCI Chemical Corporation. Provox ® C is more than 95% sodium percarbonate.

The chemical reaction of sodium percarbonate under ideal conditions (100% efficiency of reaction) in water is shown below.
The oxygen gas produced by sodium percarbonate solution in the sand specimen resulted in reduction in the degree of saturation of the sand.

### 4.2 Constitutive Parameters for Gas Generation in Sand

This section presents laboratory experiments that were conducted to determine the rate parameter, \( r \), as well as the efficiency coefficient, \( E_f \), of the chemical reaction of sodium percarbonate generating oxygen gas in sands. Details of the constitutive model for gas bubble generation were presented in Section 3.3.2. In order to complete this constitutive model, the rate parameter for the chemical reactivity of sodium percarbonate needed to be determined experimentally.

#### 4.2.1 Rate of Gas Generation in Sand

Laboratory experiments were conducted to determine the rate of gas generation in sands. The picture of the batch test set-up and the instrument to detect gas generation are shown in Figure 4-2. An electric conductivity probe shown in Figure 4-2 was used to detect gas generation in the pore space of a sand specimen. Electric conductivity is a function of not only the electrical resistance of the pore fluid containing ions but also the cross sectional area shared by the sand particles and the conductive pore fluid. Therefore, as oxygen gas bubbles form in the pore space, the cross section area of the pore fluid decreases and thus the electrical conductivity decreases. Consequently, measurement of the decrease in electric conductivity over time indicates the generation of oxygen gas in the pores.
Details of the use of electrical conductivity probes and the batch experiments for various concentrations of sodium percarbonate are presented in a soon to be published dissertation by Hadi Kazemiroodsari, a Ph.D. student also working on this project funded by NSF, NEESR.

In the batch tests run to investigate the rate of gas generation, 0.5% and 1% concentrations of sodium percarbonate were used, and measurements of electrical conductivity were made while the solution reacted in water and generated gas bubble in the pores of the sand specimens.

Figure 4-3 presents the electrical conductivity measurements as a function of time. Initial high readings of electrical conductivity are indicative of the presence of sodium and carbonate ions. As gas bubbles are generated, the area of the pore fluid decreases and electric conductivity decreases. Therefore during exponential generation of gas bubbles, the electrical conductivity in soil is expected to decrease exponentially. The experimental data presented in Figure 4-3 shows this decrease in electrical conductivity measured for two specimens prepared with two different initial concentrations of sodium percarbonate.
solution. As expected, the initial electrical conductivity value for 0.5% is lower than for 1.0%. The experimental data presented in Figure 4-3 was used to determine the rate parameter, r, for the chemical reaction of sodium percarbonate for the two concentrations of 0.5% and 1.0%.

![Generation of Oxygen Bubbles in Sand](image)

Figure 4-3 Electrical conductivity in sand during gas generation (a) C=0.5% (by weight) and (b) C=1.0% (by weight)

Figure 4-4 presents further explanation of the reading of the electrical conductivity. The electrical conductivity starts from an initial peak value (EC₀) at zero time and ends at
the residual electrical conductivity \( (EC_{\text{res}}) \) at the end of gas generation, as shown in Figure 4-4.

![Figure 4-4 Representation of gas bubble generation using electrical conductivity probes (0.5% concentration)](image)

Observing the exponential decrease in electric conductivity (Figure 4-4), the following equation was formulated to capture this trend.

\[
EC(t) = (EC_i - EC_{\text{res}}) \times e^{(-rt)} + EC_{\text{res}} \quad (4-4)
\]

where:

- \( EC(t) \) = electric conductivity at time \( t = t \)
- \( EC_i \) = initial (peak) electrical conductivity at \( t = 0 \)
- \( EC_{\text{res}} \) = residual electrical conductivity at the end of gas generation
- \( r \) = rate parameter
It is noted that the reduction in electric conductivity is due to gas generation by the decay of hydrogen peroxide. Therefore, $(EC_i - EC_{res})$ can be considered proportional to the initial concentration of the hydrogen peroxide, $C_0$ of Equation (4-2).

$$(EC_i - EC_{res}) = C_0$$

$(EC_i - EC_{res})$ is the remaining concentration of hydrogen peroxide at time $t$.

$$(EC_i - EC_{res}) = C(t)$$

Rewriting Equation (4-5);

$$EC(t) - EC_{res} = (EC_i - EC_{res}) \times e^{(rt)}$$

and in terms of $C$, the concentration of solute as defined in SUTRA-Bubble, Equation (4-4) can be expressed as

$$C(t) = (C_0) e^{(-rt)}$$

This leads to the conclusion that $r$ in Equation (4-4) is the same rate parameter $r$ of Equation (4-2). Using Equation (4-4) and the experimental data in Figure 4-3, values of the rate parameter, $r$ were estimated as shown in Figure 4-5: $r = 0.000133$ (per second) for 1% initial concentration and $r = 0.000083$ (per second) for 0.5% initial concentration.
Figure 4-5 Fitted equation with exponential rate parameter determined for (a) C=0.5% and (b) C=1.0%

A goodness of fit test of the fitted lines was conducted for each rate parameter. Table 4-1 shows the coefficient of determination for each data set measured. Values from 0.96 to 0.99 were calculated for coefficient of determination, which confirms a good fit for the rate parameters for 0.5% and 1% concentrations. The two rate parameters presented in Table 4-1 were used in the simulations of the experiments conducted to validate SUTRA-Bubble.
Table 4-1 Goodness of fit test results for exponential rate parameter

<table>
<thead>
<tr>
<th>Equivalent Concentration</th>
<th>Exponential Coefficient, r (1/sec)</th>
<th>Coefficient of Determination, $R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5%</td>
<td>0.0000833</td>
<td>0.96</td>
</tr>
<tr>
<td>1%</td>
<td>0.000133</td>
<td>0.99</td>
</tr>
</tbody>
</table>

**4.2.2 Efficiency of Gas Generation in Sand**

The efficiency coefficient, $E_f$, for the chemical reaction is required to adjust the design concentration of solute to run SUTRA-Bubble simulations. The efficiency factor $E_f$ was described in detail in Section 3.3 of Chapter 3.

There are a number of factors that can affect efficiency of the chemical reaction of the sodium percarbonate in water as well as in a sand specimen.

OCI Chemical Corporation states that its product Provox ® C (sodium percarbonate) has an efficiency of about 85% in generating oxygen gas in water. Oxygen generated in the pores of a sand specimen can also dissolve, thus reducing the efficiency of chemically generated free gas bubbles in the sand pores. The solubility of oxygen under 1 atm pressure and 77 °F temperature is 0.000258 (mole/liter). The percent of dissolved oxygen of the total molar concentration of generated oxygen is quite small, (0.25% - 1.0%). Therefore, it is concluded that the effect of solubility of oxygen gas on the efficiency coefficient, $E_f$, is negligible.

Table 4-2 shows the calculated values of the molar concentrations of generated oxygen for different concentrations of sodium percarbonate, computed by using Equation (4-5).

\[
n_{(O_2)} \text{ (mole/liter)} = \left( C_{SPC} \right) \times (MW_{SPC}) \times 0.75 \tag{4-5}
\]
The percent of dissolved oxygen of the total molar concentration of generated oxygen is quite small, (0.25% - 1.0%). Therefore, it is concluded that the effect of solubility of oxygen gas on the efficiency coefficient, $E_f$, is negligible.

Table 4-2  Loss due to solubility of oxygen gas under normal conditions

<table>
<thead>
<tr>
<th>Sodium percarbonate concentration (by weight)</th>
<th>Molar concentration of generated oxygen, $n_{O_2}$ (moles/liter)</th>
<th>Solubility of Oxygen, $n_{DO}$, (moles/liter) (1 atm, 77 °F)</th>
<th>Fraction of $n_{DO}/n_{O_2}$, (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5%</td>
<td>0.0239</td>
<td>0.000258</td>
<td>1.0%</td>
</tr>
<tr>
<td>1.0%</td>
<td>0.0478</td>
<td>0.000258</td>
<td>0.50%</td>
</tr>
<tr>
<td>1.5%</td>
<td>0.0717</td>
<td>0.000258</td>
<td>0.33%</td>
</tr>
<tr>
<td>2.0%</td>
<td>0.0956</td>
<td>0.000258</td>
<td>0.25%</td>
</tr>
</tbody>
</table>

The previous discussions on the efficiency of sodium percarbonate generating gas bubbles were for the chemical reaction taking place in fresh water. The efficiency of the reaction of sodium percarbonate generating oxygen bubbles in sands was also investigated. Laboratory experiments were conducted to evaluate the overall efficiency of sodium percarbonate generating gas bubbles in Ottawa sand specimens. Specimens were prepared by raining dry sand into sodium percarbonate solutions of various concentrations. As gas bubbles were generated in the pores of a specimen, solution was accumulated on top of the specimen. The volume of accumulated solution was equated to volume of gas generated. This measured volume of gas was compared with the volume of gas computed using stoichiometric coefficients of the sodium percarbonate reaction and the ideal gas law, and assuming 100% efficiency as shown in Equation (4-6).
\[
\text{Na}_2\text{CO}_3 \cdot 1.5\text{H}_2\text{O}_2 \xrightarrow{\text{in water}} 2\text{Na}^{+1} + \text{CO}_3^{2-} + 1.5\text{H}_2\text{O} \quad (\text{at the end of reaction})
\]

\[
1.5\text{H}_2\text{O}_2 \xrightarrow{\text{in water}} 1.5\text{H}_2\text{O} + 0.75\text{O}_2 \quad \text{(ideal conditions - 100\% efficiency)}
\]

\[
V_{O_2} = V_{source} \times \left[ C_{SPC} \times \rho \times \frac{1}{MW_{SPC}} \times 0.75 \times 22400 \right] \quad (4-6)
\]

where:

- \(V_{O_2}\) = volume of oxygen gas
- \(V_{source}\) = volume of solution that generates gas bubbles in the pores of a sand specimen
- \(C_{SPC}\) = design concentration of sodium percarbonate solution
- \(\rho\) = density of solution
- \(MW_{SPC}\) = molecular weight of sodium percarbonate

It is noted that \(V_{source}\) volume of solution in the pores decreased as gas bubbles were generated and pushed the solution out of the pore space, thus losing the potential gas volume that the solution would have generated in the pores. Therefore, adjustments were needed in the calculation of the source volume \(V_{source}\) which is used to determine the volume of gas produced in the pores of the specimen (Equation 4-6). Figure 4-6 shows a sketch of the sand specimen with the accumulated solution on top of the surface. Since this accumulating volume of solution on top of a specimen was changing over time, it was hard to determine a value for adjustment as a function of time. Therefore, the final value of the accumulated volume of solution was considered as a loss and was subtracted from the initial volume of solution available in the pores.
In Table 4-3 the measured volumes of gas from the laboratory experiments are compared with the computed volumes using Equation (4-6) for 100% efficiency. The results show that the efficiency of sodium percarbonate, $E_f$, generating gas bubbles in Ottawa sand ranged between 56% and 89%. An average value of efficiency $E_f = 76\%$ for the chemical reaction in the pore space of the sand specimen was deemed to be a reasonable value to use in SUTRA-Bubble.

Table 4-3  Bench top experiment output to determine efficiency of sodium percarbonate reaction in sand

<table>
<thead>
<tr>
<th>Data Set</th>
<th>CSPC</th>
<th>$V_{source}$, ml</th>
<th>$V_{O_2}$, ml (measured)</th>
<th>$V_{O_2}$, ml (Equation 4-6)</th>
<th>Efficiency, $E_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data Set 1</td>
<td>1.0%</td>
<td>163.0</td>
<td>136</td>
<td>179.7</td>
<td>76%</td>
</tr>
<tr>
<td>Data Set 2</td>
<td>1.0%</td>
<td>89.8</td>
<td>88</td>
<td>99.0</td>
<td>89%</td>
</tr>
<tr>
<td>Data Set 3</td>
<td>1.0%</td>
<td>154.3</td>
<td>96</td>
<td>170.1</td>
<td>56%</td>
</tr>
<tr>
<td>Data Set 4</td>
<td>0.5%</td>
<td>176.0</td>
<td>80</td>
<td>97.0</td>
<td>82%</td>
</tr>
<tr>
<td>Data Set 5</td>
<td>0.5%</td>
<td>132.7</td>
<td>56</td>
<td>73.1</td>
<td>77%</td>
</tr>
<tr>
<td>Data Set 6</td>
<td>0.8%</td>
<td>137.3</td>
<td>88</td>
<td>121.1</td>
<td>73%</td>
</tr>
<tr>
<td><strong>Average Efficiency</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td><strong>76%</strong></td>
</tr>
</tbody>
</table>
4.3 Constitutive Parameter for Relative Permeability of Sand

This section presents constant head permeability experiments conducted on partially saturated specimens in order to determine the relative permeability, $k_r$, in partially saturated specimens created by IPS. Equation (4-3) is repeated below, showing that the relative permeability, $k_r$, is related to the degree of saturation with an exponent of $n$ (details were provided in Section 3.2, in Chapter 3)

$$k_r = \frac{k_{PS}}{k_{FS}} = (S_w^t)^n$$

where:
- $k_{PS}$ = permeability for partially saturated soil
- $k_{FS}$ = permeability for fully saturated soil
- $S_w^t$ = total degree of saturation in SUTRA-Bubble
- $n$ = constant exponent for degree of saturation

4.3.1 Laboratory Experiments for Relative Permeability of Sand

A constant head permeability experimental test set-up was prepared to run tests on partially saturated sands created by IPS (Figure 4-7). A Plexiglas cylinder was used in which fully and partially saturated sand specimens were prepared. A fully saturated specimen was prepared by raining dry sand in the cylinder partly filled with water. A partially saturated sand specimen was prepared by raining a mixture of dry sand and sodium percarbonate powder. The void ratio and degree of saturation of a specimen were determined by phase relations using the height and volume measurements taken from the specimen. When a fully or partially saturated specimen was ready to be tested, a saturated
porous stone was placed on top of the specimen and the column was sealed airtight with its metal top. De-aired water was circulated to saturate the gap between the porous stone and the top of the column until the top relief valve was saturated.

![Experimental Setup](image)

**Figure 4-7** The experimental set up for constant head permeability tests

The elevation difference between the constant level of inflow source and the outflow drain was computed to determine the flow gradient. The height of the stand for inflow source was changed in order to create various levels of hydraulic gradients in the soil. The inflow and outflow of the de-aired water were recorded at every 15 seconds. Permeability values were then computed using the measured flow rates and hydraulic gradients. The results from tests on five different specimens, (two fully saturated and three partially saturated) are presented in Table 4-4.
As noted in Table 4-4 the void ratios of the fully saturated specimens were the same (0.71), whereas the three partially saturated specimens had slightly different void ratios. Since relative permeability is computed as the ratio of permeabilities of partially and fully saturated specimens, having the same void ratio, the permeability of a fully saturated specimen corresponding to the void ratio of a partially saturated specimen was needed. This was obtained by adjusting the average permeability value of the fully saturated specimens with void ratio of 0.71, to correspond to the void ratios of the partially saturated specimens.

This adjustment was done using Kozeny-Carman relationship between soil permeability and void ratio that is shown in Equation (4-7).
\[ \frac{k_1}{k_2} = \frac{e_1^3}{e_2^3} \frac{1}{(1 + e_1)} \quad \text{(Kozeny-Carman)} \]  

(4-7)

In Equation (4-7), \( k_1 \) was considered the permeability of a fully saturated specimen with void ratio of 0.71. The value of \( k_1 \) was assigned as 0.049 cm/sec, which was computed as average of the seven fully saturated tests (Table 4-4), which all had void ratio of 0.71. Again in Equation (4-7), \( k_2 \) is then the permeability a fully saturated specimen adjusted to correspond to void ratio of \( e_2 \). The adjusted fully saturated permeability values for each void ratio are shown in Table 4-5.

Table 4-5 Average saturated permeability values, \( k_{FS} \) in Equation (4-3) corrected for void ratio

<table>
<thead>
<tr>
<th>Void Ratio</th>
<th>Average ( k_{FS} ) (cm/s) (adjusted for void ratio)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.71</td>
<td>0.049</td>
</tr>
<tr>
<td>0.77</td>
<td>0.060</td>
</tr>
<tr>
<td>0.80</td>
<td>0.066</td>
</tr>
<tr>
<td>0.75</td>
<td>0.056</td>
</tr>
</tbody>
</table>

Relative permeability, \( k_r \) values for the partially saturated specimens were then determined by normalizing the measured permeability values for each partially saturated specimen with their corresponding adjusted fully saturated permeability. Relative permeability values computed for each saturation level are tabulated in Table 4-6.
Table 4-6 Relative permeability values

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Degree of Saturation</th>
<th>Gradient, i</th>
<th>Permeability, cm/s</th>
<th>Void Ratio</th>
<th>kr (k_{PS}/k_{FS})</th>
</tr>
</thead>
<tbody>
<tr>
<td>FS4-1</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.84</td>
<td>0.038</td>
<td>0.71</td>
</tr>
<tr>
<td>FS4-2</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.48</td>
<td>0.051</td>
<td>0.71</td>
</tr>
<tr>
<td>FS4-3</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.61</td>
<td>0.050</td>
<td>0.71</td>
</tr>
<tr>
<td>FS5-1</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.63</td>
<td>0.053</td>
<td>0.71</td>
</tr>
<tr>
<td>FS5-2</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.40</td>
<td>0.050</td>
<td>0.71</td>
</tr>
<tr>
<td>FS5-3</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.22</td>
<td>0.044</td>
<td>0.71</td>
</tr>
<tr>
<td>FS5-4</td>
<td>Fully Saturated (FS)</td>
<td>1.00</td>
<td>0.22</td>
<td>0.044</td>
<td>0.71</td>
</tr>
<tr>
<td>PS3-1</td>
<td>Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.66</td>
<td>0.050</td>
<td>0.77</td>
</tr>
<tr>
<td>PS3-2</td>
<td>Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.63</td>
<td>0.048</td>
<td>0.77</td>
</tr>
<tr>
<td>PS3-3</td>
<td>Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.43</td>
<td>0.049</td>
<td>0.77</td>
</tr>
<tr>
<td>PS3-4</td>
<td>Partially Saturated (PS)</td>
<td>0.90</td>
<td>0.23</td>
<td>0.048</td>
<td>0.77</td>
</tr>
<tr>
<td>PS2-1</td>
<td>Partially Saturated (PS)</td>
<td>0.66</td>
<td>0.64</td>
<td>0.028</td>
<td>0.80</td>
</tr>
<tr>
<td>PS2-2</td>
<td>Partially Saturated (PS)</td>
<td>0.65</td>
<td>0.44</td>
<td>0.029</td>
<td>0.80</td>
</tr>
<tr>
<td>PS2-3</td>
<td>Partially Saturated (PS)</td>
<td>0.66</td>
<td>0.22</td>
<td>0.024</td>
<td>0.80</td>
</tr>
<tr>
<td>PS2-4</td>
<td>Partially Saturated (PS)</td>
<td>0.66</td>
<td>0.89</td>
<td>0.027</td>
<td>0.80</td>
</tr>
<tr>
<td>PS4-1</td>
<td>Partially Saturated (PS)</td>
<td>0.49</td>
<td>1.17</td>
<td>0.016</td>
<td>0.75</td>
</tr>
<tr>
<td>PS4-2</td>
<td>Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.90</td>
<td>0.020</td>
<td>0.75</td>
</tr>
<tr>
<td>PS4-3</td>
<td>Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.66</td>
<td>0.019</td>
<td>0.75</td>
</tr>
<tr>
<td>PS4-4</td>
<td>Partially Saturated (PS)</td>
<td>0.49</td>
<td>0.43</td>
<td>0.023</td>
<td>0.75</td>
</tr>
</tbody>
</table>

The computed values of relative permeability are plotted as a function of degree of saturation in Figure 4-8. Included in the figure is the relationship proposed by Brooks and Corey with n exponent 3 for clean sands (1964), kr = (S_o^3). The data appears to fit better when kr = (S_o^n)^3. Therefore, the value of 2 for n was used in the constitutive model for relative permeability in SUTRA-Bubble.
Figure 4-8 Relative permeability of Ottawa sand as a function of degree of saturation
Chapter 5

Validation of SUTRA-Bubble with Laboratory Experiments

5.1 Overview

In order to validate SUTRA-Bubble, an experimental test set-up was designed and manufactured, which enabled small scale implementation of Induced Partial Saturation (IPS) in a laboratory prepared sand specimen. The experiment involved injection of sodium percarbonate solution into a relatively large (91cm x 13.5 cm x 55 cm), saturated sand specimen with controlled pressure and chemical concentration, leading to a certain zone of partial saturation. Measurements were made of inflow and outflow of solution, pressures in the specimen during injection of solution, transport and reactivity of solution into the sand specimen, and degree of saturation in the specimen. Two comparable tests were conducted with different concentrations, and SUTRA-Bubble simulations for these two tests were made and compared with the experimental measurements for the purpose of validating SUTRA-Bubble. Comparisons of the SUTRA-Bubble predictions were made with the three general sets of experimental test results:

1. Flow and pressure during injection
2. Transport of solution
3. Degree of saturation

This chapter first presents the experiment set-up and the test procedures, followed by the results from the two tests (TEST 1 and TEST 2). The chapter then presents the SUTRA-Bubble simulation input and results, including three-dimensional (3D) outputs of concentration of solution, and degree of saturation. Finally, the predictions of SUTRA-
Bubble simulations for both tests are compared with the experimental measurements, showing good agreement between the experimental and SUTRA-Bubble results.

## 5.2 Laboratory Experiments

An experimental test set-up was designed, which allowed injection of sodium percarbonate solution into a sand specimen with controlled pressure and chemical concentration to create a partially saturated zone in the sand specimen. A relatively large sand specimen was prepared in a glass tank instrumented to conduct these injection experiments (Figure 5-1). A glass tank was preferred in order to visually observe from the sides of the tank the partially saturated zone.

![Figure 5-1 Sand specimen in glass tank](image)

Figure 5-1 Sand specimen in glass tank

Figure 5-2 shows the entire set-up which includes; a glass tank filled with the sand specimen and instrumented with electrical conductivity probes and pore water pressure...
transducers along with relevant data acquisition systems, a Mariotte bottle which is the source for constant pressure injection of sodium percarbonate solution, and a PVC solution injection tube with a gas relief valve on top. Pressure transducers were used to measure the pore water pressures in the sand specimen during injection, and electric conductivity probes were used to monitor the transport process of the chemical solution, and to estimate the degree of saturation at various locations within the specimen.

![Figure 5-2 Set-up for IPS experiment in glass tank](image)

**5.2.1 Test Set-up and Procedure**

The glass tank experiment was repeated twice. In both tests, identical procedures were followed with a difference only in the concentration of the injected solution. In TEST 1, the concentration was about 1% and in TEST 2 0.5% by weight. The reason for
performing two tests was to observe the effect of change in concentration. Details of the test set-up and procedure follow.

Procedure for preparation of fully saturated sand specimen:

**Step 1:** In a specially manufactured glass tank (91cm x 13.5 cm x 60 cm), pore water pressure transducers and electrical conductivity probes were placed at desired locations as shown in Figure 5-3. De-aired water was produced for the preparation of fully and partially saturated sand specimens.

**Step 2:** An open-ended plastic tube (2.3 cm in diameter), with its tip covered with geotextile, was placed 30 cm from the bottom of the tank (approximately 25 cm below the eventual surface of the sand specimen). Efforts were made to ensure that the tip of the injection tube was level to maintain symmetry of fluid injection.

![Figure 5-3 Glass tank and instrumentation and injection tube before specimen preparation](image)

**Step 3:** A fully saturated loose sand specimen was prepared by wet pluviation. The technique involved raining dry Ottawa sand into de-aired water in the glass tank.
Approximately 100 kgs of dry Ottawa sand was poured into de-aired water for about 4-5 hours. This technique resulted in a loose sand specimen with a height of 55 cm and porosity of 0.4-0.42 (Figure 5-4). Properties of the specimen such as porosity, initial degree of saturation (expected to be 100%) were determined through phase relations using height measurements of the water, and the specimen as well as weight of the sand rained.

Step 4: Inflow of water first and then solution was provided at a constant head difference using a Mariotte bottle placed at about of 172.6 cm from the floor, thus creating 27.15 cm head difference at the tip of the injection tube assuming no loss of head due to flow (Figure 5-5). The Mariotte bottle was manufactured out of Plexiglas with a 2.3 cm diameter outlet (same as the size of the injection tube) to supply enough flow into the sand specimen. The bottle was able to supply approximately 16 liters of fluid during a test.
Figure 5-5 Mariotte bottle hanging on the wall supplying constant head flow

Figure 5-6 (a) shows the picture of the Mariotte bottle designed and manufactured for constant head injection. The concept is widely used to create constant pressure of water or any fluid by the help of the elevation difference. The sketch of a typical Mariotte bottle is shown in Figure 5-6 (b). It is a bottle where there is only one inlet (standpipe) and one outlet. The inlet is a standpipe with the tip at atmospheric pressure and thus the pressure in the tank is always atmospheric even if the water level drops in the bottle. This enables the constant head outflow from the bottle with a head equivalent to elevation difference between the tip of the standpipe and the tip of the outlet (h in Figure 5-6 (b)), which in the experiment is the tip of the injection tube.
The Mariotte bottle was tested to see if it was able to apply the measured elevation difference at the tip of the injection tube without any loss. Figure 5-7 shows a sketch of the small scale test set-up. The end of the flexible tube was connected to the injection tube. When the injection tube got completely saturated, the tip of the injection tube became the outlet of the Mariotte bottle. Thus, the constant head applied to the sand specimen became the elevation difference from the tip of the standpipe in Mariotte bottle and the constant free water level on top of the specimen which is labeled as $\Delta H$ (MB) in Figure 5-7. At the tip of the injection tube, the applied head difference $\Delta H$ (TIP) theoretically is equal to $\Delta H$ (MB), if there is no loss of head in the tubes.
ΔH (TIP) was measured using two pore pressure transducers, where one was inserted inside the injection tube and the other in the sand right outside the injection tip.

ΔH (MB) = 35 cm

Figure 5-7 Sketch of the test for testing the possible head loss in Mariotte bottle set-up

Figure 5-8 Pore water pressures measured inside and outside the injection tube
Figure 5-8 shows a measured head difference inside the injection tube of 34 cm (ΔH (TIP)), when the elevation difference was 35 cm (ΔH (MB)). Therefore, the loss in head difference was determined to be small (approximately 1.0 cm). Figure 5-8 also shows that the pressure head drops significantly in sand even very close to the tip of the injection tube, which demonstrates that the loss in the tube is quite negligible when compared to the loss in sand.

Step 5: Mariotte Bottle was used at the start of a test to inject clean de-aired water to ensure saturation of the specimen and to measure flow rate in a fully saturated specimen for later comparison with SUTRA-Bubble predictions. This comparison helped to back-calculation permeability of the fully saturated specimen.

After injection of clean water, the Mariotte bottle was used to inject sodium percarbonate solution. The solution was prepared by mixing a predetermined amount of powder and de-aired water to achieve a desired concentration. The mixing was done using magnetic stirrer for approximately 5 minutes.
Procedure for injection of sodium percarbonate solution

Flow measurements

The Mariotte bottle was first filled with de-aired water then sodium percarbonate solution for an injection test. Before the start of the injection test, the injection tube was saturated with clean water. A relief valve was attached to the injection tube in order to release the air inside the injection tube. During solution injection, because of the short duration, the gas accumulated in the injection tube was not substantial and thus the relief valve was rarely used.

Inflow and outflow water weights were measured by reading the weights of the Mariotte bottle and the bucket that collected the outflow water from the top of a specimen. Figure 5-10 shows the measurement set-up for the inflow and outflow quantities. During injection of clean water and solution, measurements of inflow and outflow were recorded every 30 seconds. In the case of injection of solution, after the end of injection outflow of the fluid displaced by the generated gas in the pores of the sand specimen was recorded.

![Figure 5-10 Measurements of inflow and outflow](image)

Intelligent PC-30000 Model scale
30000 gr capacity with 1 gr precision
**Pressure measurements**

Five miniature pore water pressure transducers were placed in the glass tank to measure pore pressures at different locations in the sand specimen during the injection process. Two different brands of pressure transducers were used: two (2) were Druck PDCR 81 and three (3) were Kulite XCL-11-250, as shown in Figure 5-11. The concept design of the two transducers are very similar. They both include a porous stone in front of a membrane for pressure sensing. The difference in the two types of transducers is in their porous stones. The porous stone at the tip of Druck PDCR 81 is finer than that of the Kulite brand.

![Image of pore pressure transducers](image)

Figure 5-11 Pore pressure transducers used in laboratory experiments

The stability of pore pressure transducers in fully saturated sand specimens was quite good, however the transducers lost their stability as the chemical solution was injected into the specimen and created oxygen gas bubbles. The details of the performance of pore pressure transducers during sodium percarbonate injection can be found in soon to be published dissertation by Hadi Kazemiroodsari.
The two pore pressure transducers (Druck PDCR 81) were placed immediately next to the tip of the injection tube to check whether the flow was symmetric. The other three transducers (Kulite XCL-11-250) were placed away from the injection tube to observe how the pressures were distributed within the specimen.

**Electrical conductivity measurements for detecting transport of solution and estimation of degree of saturation**

The use of electrical conductivity measurements to study induced partial saturation by injection of sodium percarbonate solution is described in the dissertation soon to be completed by Hadi Kazemiroodsari. In the glass tank experiments conducted to validate SUTRA-Bubble, 12 electrical conductivity probes were used to detect the transport of the solution and to estimate the degree of saturation in the sand specimen at the locations of the probes.

Figure 5-12 shows a typical electrical conductivity probe and recording meters used in the glass tank experiments.

![Figure 5-12 Electrical conductivity probe and recording meters](image)
Electrical conductivity is a measure of the ability of a medium to conduct electrical current. Therefore, electrical conductivity of a medium increases with the presence of ions. Sodium percarbonate solution has ions of sodium and carbonate in addition to hydrogen peroxide, which is the source of oxygen gas. Electrical conductivity in a sand rapidly increases to a certain peak value with the arrival of sodium percarbonate solution at a probe location. Therefore, the electrical conductivity probes could detect the transport of sodium percarbonate solution in the sand specimen.

Electrical conductivity not only relates to arrival of ions in solution that is in between two electrodes, but also the cross sectional area of the conductive fluid in between the two electrodes. As oxygen gas bubbles are generated in the pore space, the area of conductive pore fluid decreases, leading to a decrease in electrical conductivity. It is noted that this decrease in electrical conductivity can be related to the local change in degree of saturation. Archie’s law expresses electric resistivity as a function of a number of parameters, as shown in Equation (5-1). Electrical conductivity is the inverse of resistivity (Equation 5-2). Typical decrease in electrical conductivity during gas generation is shown in Figure 5-13.

\[
\rho = a \times \rho_w \times \phi^{-m} \times S^{-n} \tag{5-1}
\]

- \(\rho\) = Resistivity of sand
- \(a\) = tortuosity factor
- \(\rho_w\) = Resistivity of brine
- \(\phi\) = Porosity
- \(S\) = degree of saturation
- \(m\) = Cementation exponent (1.8-2 for consolidated sandstones)
- \(n\) = Saturation exponent (for clean unconsolidated and for consolidated sands 2)
Conductivity ($\sigma$) is defined as the inverse of resistivity $\sigma = \frac{1}{\rho}$

$$\sigma = 1/(a \times \sigma_w \times \varphi^m \times s^n) \quad (5-2)$$

$\sigma$: Conductivity of sand

$\sigma_w$: Conductivity of brine

Figure 5-13 Methodology to estimate degree of saturation using Archie’s law

The rise in electric conductivity is due to arrival of ions. The decrease in electric conductivity is attributed to gas bubbles generated in the sand pores. At the location of a probe, the time it takes to reach its maximum concentration (peak electrical conductivity value) is relatively short (approximately 1 – 3 minutes). Therefore, it is assumed that during this time, the amount of gas generated is negligible compared to the total gas generation (from point P to point R in Figure 5-13). This assumption is validated by comparing inflow and outflow values during the short duration of injection of solution which is presented in Section 5.4.1.1. Degree of saturation can be estimated by:

$$S = \sqrt{\frac{\sigma_R}{\sigma_P}} \quad (5-3)$$

in which P and R are the electrical conductivity values at those points.
Twelve electrical conductivity probes were placed in selected locations in the glass tank before specimen preparation. Two of them were placed right at the tip of the injection tube to observe the symmetry of the transport. The locations in the sand specimen of the pore pressure transducers and electric conductivity probes are presented in Figure 5-14.

![Figure 5-14 Locations of instruments for both Test 1 and Test 2](image)

**Probe for measuring concentration of solution**

A chemical solution with a desired concentration was prepared by mixing de-aired water and sodium percarbonate by weight. To ensure that the solution indeed had the desired concentration, a Brix probe (Pen-Pro Pen refractometer) was used. This probe is a product of ATAGO ® U.S.A Inc. and measures the concentration of dissolved solids in a chemical solution. The probe is a light refractometer which can measure the change in specific gravity of a solution and determine its mass concentration.
The Brix probe was used to confirm the concentration of the solution prior to injection into the sand specimen. In addition, the probe was used to measure the concentration within the specimen by sampling pore fluids using injection needles at various locations.

Figure 5-15 shows the Brix probe and the sampling tools for extracting the solution at different depths from the sand specimen. A 30 cm long needle was used along with a syringe to extract the solution from the pore space of the sand specimen. The sampling of 30 cm below the sand surface was not possible therefore only the EC probe locations at or above the injection tip were tested by the Brix probe.
High resolution digital images to detect existence of gas bubbles

A digital imaging set-up was prepared to capture the zone of partial saturation within the specimen. The set-up includes a high resolution digital camera, a 105 mm micro lens, two LED lights pointed to the sample at approximately a 45 degree angle. Figure 5-16 shows the digital imaging set-up with its components. The 105 mm micro lens is sharp enough to capture images of gas bubbles as distinguished by their shines with the help of pointed LED lights. Digital images were taken at locations within partially and fully saturated zones to confirm the extent of the partial saturation zone.

Figure 5-16 Digital camera set-up to capture gas bubbles trapped in the sand pores

In summary, a laboratory test set-up was designed that enabled the injection of sodium percarbonate solution with controlled pressure and concentration of solution in a large sand specimen. During injection of solution, flow and pressure measurements were made to determine the flow parameters during injection such as flow rate of injection and average permeability of the sand specimen. Moreover, electrical conductivity measurements were made during and after injection in order to detect the transport of sodium percarbonate solution as well as the reduction in the degree of saturation as a result
of gas generation. In addition, a Brix probe was used to measure the concentration of the solution to detect the transport of the solution.

Two complete tests were performed (TEST 1 and TEST 2). The only differences between the tests were chemical concentration and a slight difference in void ratios of the two specimens.

Table 5-1 summarizes the injection parameters for TEST 1 and TEST 2.

Table 5-1 Parameters of injection of sodium percarbonate solution in glass tank experiments

<table>
<thead>
<tr>
<th>Test</th>
<th>e</th>
<th>Water inj.</th>
<th>IPS inj.</th>
<th>Depth of inj. tube</th>
<th>Inj. pressure – ΔH (TIP)</th>
<th>Inj. duration</th>
<th>Injection Conc. C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 1</td>
<td>0.69</td>
<td>25.5 cm</td>
<td>25.5 cm</td>
<td>26 cm</td>
<td>26 cm</td>
<td>5 min</td>
<td>0%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1%</td>
</tr>
<tr>
<td>Test 2</td>
<td>0.72</td>
<td>25.5 cm</td>
<td>25.5 cm</td>
<td>26 cm</td>
<td>26 cm</td>
<td>13 min</td>
<td>0%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.5%</td>
</tr>
</tbody>
</table>
5.2.2 Test Results

In this section, three sets of experimental test results are summarized which will later be used to compare with similar sets of results from SUTRA-Bubble for validation. The three sets of results are:

1. Flow and pressure during injection
2. Transport of chemical solution
3. Degree of saturation

Results from TEST 1 are presented and discussed in detail. Results from TEST 2 are presented and compared with the results from TEST 1 to confirm observations and conclusions.

5.2.2.1 TEST 1 Results

5.2.2.1.1 Flow and Pressure during Injection – TEST 1

Results of inflow and outflow during injection of both clean water and sodium percarbonate solution for TEST 1 are presented in Figure 5-17. The cumulative inflow and outflow of clean water are presented in Figure 5-17 (a). The rate of both inflow and outflow were constant during injection. This indicated that the Mariotte bottle was able to apply constant pressure during the injection process.
The average flow rates (q\text{ave}) of the inflow (1944 gr/min) and the outflow (1892 gr/min) were similar. The slight difference between inflow and outflow was due to the time lag of outflow, which is attributed to the geometry of drains on the side of the glass tank (Figure 5-10). This difference was also observed in the first two minutes of solution injection.
however the outflow caught up with the inflow after 3 minutes. The final values of cumulative flow for both inflow and outflow were the same showing no storage in the sand specimen.

The cumulative inflow and outflow during injection of the sodium percarbonate solution is presented in Figure 5-17(b). Slight reduction in the rate of both inflow and outflow was observed and it was noted that both followed the same decreasing trend. This reduction is associated with gas bubbles being generated in the geotextile which was placed at the tip of the injection tube in order to prevent intrusion of sand into the tube. The open area for inflow was reduced by the gas bubbles that were stuck in the fabric of the geotextile. This reduction in the open area for flow led to the reduction in the rate of inflow. Outflow was consistent with inflow. Another possible explanation is change in soil permeability due to partial saturation created during injection. However the injection duration (13 minutes) was too short to generate enough gas bubbles in the sand to affect the inflow.

In addition to flow measurements, pore water pressures were measured in the sand specimen at the locations of the 5 pore pressure transducers (PPT) used. The locations of the transducers in the sand specimen along with the results of each transducer during injection of clean water and solution are presented in Figure 5-18.
Figure 5-18 (a) Locations of PPT’s (b) PPT measurements during water injection, (c) PPT measurements during injection of sodium percarbonate solution for TEST 1
All PPT’s measured hydrostatic pressures consistent with their depths. Similar to flow measurements in clean water, the pore pressure data from all 5 PPT’s during clean water injection also confirmed that the injection pressure was constant (Figure 5-18 (a)). The pressure transducers recorded the excess pressures due to flow during injection of both clean water and solution. The head difference relative to the phreatic line, which is the top of the specimen, \( \Delta H \), was measured by all PPT’s. PPT1 and PPT2, which were very close to the tip of the injection tube, both measured the head difference as 20.5 cm when the head difference applied at the tip of the injection tube relative to the phreatic line, \( \Delta H(TIP) \), was 26 cm. The flow was symmetric since both transducers measured the same head difference on both sides of the injection tube. The head differences measured by PPT3 (about 9 cm), PPT4 (about 7 cm), and PPT5 (about 5 cm) were a lot smaller than PPT1 and PPT2 as expected since they were located farther away from the injection tube.

The pressures measured by the PPT’s during injection of sodium percarbonate solution are presented in Figure 5-18 (c). Similar to the clean water injection case, all of the PPT’s measured hydrostatic pressures consistent with their depths in the specimen. It is noted that the excess pore pressures measured by all PPT’s during injection showed the reduction during injection of the solution similar to flow measurements shown in Figure 5-17 (b).

5.2.2.1.2 Transport of Chemical Solution– TEST 1

Measurements of electrical conductivity were made using the 12 electrical conductivity probes (EC) during and after the injection of sodium percarbonate solution. The locations of the 12 probes are presented in Figure 5-19 (a). Readings of electrical
conductivity during the 13 minutes of injection of sodium percarbonate solution are presented in Figure 5-19 (b).

Figure 5-19 (a) Locations of electrical conductivity probes (b) Electrical conductivity values measured at 12 probe locations during 13 minute injection of solution for TEST 1
The electrical conductivity values measured by probes EC1 through EC9 increased in a relatively short time (within 13 minutes). The probes EC10 through EC12 recorded peak values at later times, because of their farther distances from the injection tube. It is noted that the peak values of electrical conductivity are similar for all probes (2.8 to 3.5 mS/cm) indicating concentration of solution at these locations are similar. The peak values appear to decrease with increasing distance of the probe which may be associated to the possible decrease in concentration of solution with increasing distance.

To determine the size of the zone of influence of the injection, results of the electrical conductivity at selected locations of the probes were superimposed on the picture of the sand specimen, as shown in Figure 5-20. The times of the peak values demonstrate the arrival of the maximum concentration of the solution at the probe locations. The arrival times at each probe are consistent with their distances from the injection tube.

Figure 5-20 Selected results of electrical conductivity (15 minute) superimposed on the picture of the sand specimen
As expected, the arrival times at EC1 and EC2 were immediate since they were very close to the tip of the injection tube. The arrival times at the other probe locations away from the injection tube were about 2 minutes at EC6 (∼10 cm away from injection), about 6 minutes at EC4 and EC9 (∼20 cm away from injection), and about 12 minutes at EC8 (∼25 cm away from injection). There was no evidence that the solution arrived at the locations of EC10 (∼36 cm away from injection) and EC11 (∼35 cm away from injection) during the measurement period (13 minutes).

Based on the analysis of the electrical conductivity data, it was concluded that the boundary for the zone of influence of injection was somewhere between probes EC9 and EC11 in the shallow part of the specimen, and EC8 and EC10 near the bottom of the specimen. Also, the symmetric injection of solution is confirmed by the similar arrival times at the probes on each side of the injection tube. Assuming a circular shape for the zone of influence of the concentration of solution, the radius for this zone is determined to be about 25 cm.

In addition to electrical conductivity measurements, concentrations of dissolved solids were measured using the Brix probe. Table 5-2 shows the measured values, which were very consistent with the target concentration of 1% (by weight). The results presented in Table 5-2 confirm the arrival of sodium percarbonate solution at the locations of the probes EC1 through EC9. The table does not include results from probe locations that were deeper than 30 cm (EC4 and EC8) due to the length limitation of the sampling needle.
Table 5-2  Brix probe measurements of sodium percarbonate concentration for TEST 1

<table>
<thead>
<tr>
<th>EC Probe</th>
<th>Distance from injection, cm</th>
<th>Brix Probe reading</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC1</td>
<td>0</td>
<td>0.9%</td>
</tr>
<tr>
<td>EC2</td>
<td>0</td>
<td>1.0%</td>
</tr>
<tr>
<td>EC3</td>
<td>10</td>
<td>1.0%</td>
</tr>
<tr>
<td>EC5</td>
<td>10</td>
<td>1.0%</td>
</tr>
<tr>
<td>EC6</td>
<td>10</td>
<td>1.1%</td>
</tr>
<tr>
<td>EC7</td>
<td>15</td>
<td>1.1%</td>
</tr>
<tr>
<td>EC9</td>
<td>20</td>
<td>1.0%</td>
</tr>
</tbody>
</table>

5.2.2.1.3 Degree of Saturation – TEST 1

The measured electrical conductivity values in the sand specimen were plotted for 10 hours to identify the zone of partial saturation, and to estimate the degree of saturation in the partial saturation zone, (Figure 5-21).

Figure 5-21 Electrical conductivity measured during injection and gas generation-TEST 1
The probes located within the zone of influence EC1 through EC9 recorded the reduction in electrical conductivity due to gas generation. The electric conductivity values were almost constant after 2 hours.

The electric conductivity readings at probes that were outside the zone of influence (EC10 and EC11) did not show expected trend of electrical conductivity in sand. They recorded increases in electric conductivity long after injection. The arrival at probe EC11 was approximately 1.5 hours after injection and arrival at probe EC10 was approximately 4 hours after injection. The change in electrical conductivity at these locations were due to movement of sodium and carbonate ions because the arrival of solution at these probes occurred after nearly all the hydrogen peroxide had already decomposed. Therefore, it was assumed that there was no change in degree of saturation at these probes (EC10 and EC11).

Results of 12 hour measurements of electric conductivity at selected probe locations were also superimposed on the enhanced image of the sand specimen as shown in Figure 5-22. The image was taken after the gas generation was complete. Enhancements were made to the image in order to show the distinction of the partial saturation zone. The partial saturation zone appears in lighter color in the picture. Figure 5-22 shows that EC10 and EC11 are outside the partial saturation zone. The visual observation of the partially saturated zone matched well with the probe estimations. The probes from EC1 through EC9 helped define the size of the partially saturated zone.
Figure 5-22 Selected results of electrical conductivity (12 hours) superimposed on enhanced picture of the sand specimen

Measurements of the electric conductivity for 10 hours were also used to compute the change in degree of saturation in the specimen. The method followed to estimate the degree of saturation using Archie’s law was explained in Figure 5-13 and quantified in Equation (5-3).

The degree of saturation values calculated from the results of the probes in the zone of influence, which are probes EC1 through EC9, are presented in Figure 5-23.

The rates of decrease in the degree of saturation at most of the probes were quite similar except at probes EC1 and EC2, located near the tip of the injection tube. This was attributed to the boundary effect caused by the plastic injection tube around these probes.
The final values of degree of saturation at the end of reaction estimated based on the electric conductivity measurements are also presented on the enhanced picture of the sand specimen showing the partial saturation zone in Figure 5-24. The degree of saturation from measurements from 9 probes ranged between 59% and 73%. There was no correlation between the degree of saturation and the distances of the probes from the injection tube. The average value of degree of saturation from these probes was 65%. The variability in the estimated degree of saturation values can be attributed to variability in soil density, and to the accuracy of the method to estimate the degree of saturation.

This average value of degree of saturation from probe measurements in the partially saturated zone was also compared with degree of saturation measured in a batch experiment conducted with 1% concentration of solution to measure the rate of gas generation. The batch experiment is presented in the dissertation soon to be completed by Hadi Kazemiroodsari. The degree of saturation measured in the batch experiment was 62%,
which is in good agreement with the average degree of saturation obtained from the 9 probe measurements, 65%.

The Figure 5 24 also demonstrates the partially saturated zone with a line determined by visual observation. The radius of the partial saturation zone is determined to be about 30 cm based on the visual observations.

![Figure 5-24 Picture of partially saturated sand specimen –TEST 1](image)

In addition to the picture showing the whole specimen, micro images of the sand were taken to visually observe the soil/fluid/bubbles matrix. The digital images were enhanced using Photoshop CS3 Extended in order to identify the oxygen gas bubbles. The enhanced images of fully and partially saturated portions of the specimen are presented in Figure 5-25. The oxygen gas bubbles appear shiny in the image taken from the partially saturated zone in the sand specimen.
Figure 5-25 Digital images of fully and partially saturated specimens showing gas bubbles for TEST 1

Further estimation of degree of saturation within the partially saturated zone was made using the results of outflow measurements. The measurements of outflow at 10 hours test duration are presented in Figure 5-26. The volume of oxygen gas generated in the pore space of the sand specimen during chemical reaction led to outflow of pore fluid from the top of the specimen. The difference between outflow and inflow measurements represents the total volume of oxygen gas generated. As shown in Figure 5-26, the fluid flowing out of the specimen, indicating gas bubble generation, 2 hours after the start of the test was very small. This indicates completion of reaction and generation of gas bubbles. This observation was also confirmed by the electrical conductivity results that were shown in Figure 5-23.
An average degree of saturation in the zone of partial saturation achieved at the end of reaction was calculated from outflow measurements. This method has two sources of errors; inability to efficiently collect water from the surface of the sand specimen and the determination of the size of the partially saturated zone relative to the entire specimen. In order to quantify the error due to the size estimation of the partially saturated zone, a range of percent volume of the partially zone was assumed which was between 55 to 60% of that of entire specimen determined using the grid made on the glass tank. The average degree of saturation within the partially saturated zone was then calculated as follows:

![Graph showing cumulative flow and volume of gas over time.](image)
Average degree of saturation

\( S_{AVE} \) in the zone of partial saturation using outflow measurements:

\[(\text{Outflow} - \text{Inflow}) \@ 10 \text{ hours} = (\Delta V_{\text{water}}) = (V_{\text{bubble}}) = 4292 \text{ cm}^3\]

e = 0.69

n = 0.41

\( V_t = 65874 \text{ cm}^3 \)

\((V_v)\) for entire specimen = n \((V_v) = 0.41 \times 65874 = 27008 \text{ cm}^3 \)

\((V_v)\) for partially saturated zone = (0.55 to 0.60) \times (V_v) for entire specimen

0.55 \times 26895 = 14855 \text{ cm}^3

0.60 \times 26895 = 16205 \text{ cm}^3

\( (S_{AVE}) = (V_v - V_{\text{bubble}}) / V_v \)

for 55% zone of partial saturation \((S_{AVE}) = (14855-4292)/14855 = 0.71 = 71\% \)

for 60% zone of partial saturation \((S_{AVE}) = (16205-4292)/16205 = 0.74 = 74\% \)

The average degree of saturation calculated from outflow measurements is in the range of 71 to 74%, which is above the average value of degree of saturation obtained from probe measurements in glass tank, as well as the degree of saturation measured in the batch experiments (65%). This confirms the likely error described earlier in outflow measurements due to inability to collect water efficiently from the surface of the specimen is substantial. Slow and small volume of outflow generated after 2 hours was difficult to capture by the drain system of the experiment set-up and measure accurately its weight.

It is concluded that the degree of saturation within the partially saturated zone achieved in the specimen of TEST 1 was about 65%.
5.2.2.2 TEST 2 Results

To confirm the experimental results and observations from TEST 1, a second test was conducted in which all parameters and procedures were identical to TEST 1 except the concentration of the fluid was reduced from 1% to 0.5%. Table 5-1 summarizes injection parameters used in TEST 2.

In this section results from TEST 2 are presented in the same format as was presented for TEST 1.

5.2.2.2.1 Flow and Pressure during Injection – TEST 2

The inflow and outflow measurements during injection of both clean water and solution for TEST 2 are presented in Figure 5-27 (a) and (b). Similar to TEST 1, linear trends in the cumulative inflow and outflow during clean water injection were observed. The flow rates for inflow (2400 gr/min) and outflow (2420 gr/min) were higher in TEST 2 compared to TEST 1 (1944 gr/min and 1892 gr/min). This difference in flow rates is attributed to the difference in the void ratios, and therefore the permeabilities of the two specimens. The void ratio of TEST 2 specimen was 0.72 and TEST 1 specimen was 0.69, indicating that the specimen in TEST 2 is slightly looser than the specimen in TEST 1.

During injection of solution, decrease in the rate of both inflow and outflow was also observed in TEST 2. However, the decreasing trend was more pronounced in TEST 2 than in TEST 1. This could be because more gas bubbles were stuck at the tip of the injection tube during injection in TEST 2. It is noted that after the injection tube was saturated with the solution, there was a 10 minute inadvertent delay in the start of injection.
Similar to TEST 1, the inflow and outflow followed the same trend during injection and they were the same at the end of injection, indicating that gas generation within the specimen was insignificant.

![Figure 5-27 Inflow and outflow during (a) water injection and (b) sodium percarbonate solution injection for TEST 2](image-url)

Pressures measured in TEST 2 during injection of clean water and subsequent injection of solution are presented with the locations of the instruments in Figure 5-28. The results during injection of clean water of TEST 2 are very similar to the results of TEST 1.
Injection of water – TEST 2
\[ \Delta H (TIP) = 26 \text{ cm} \]

Injection of solution – TEST 2
\[ \Delta H (TIP) = 26 \text{ cm} \]

Figure 5-28 (a) Locations of PPT’s (b) PPT measurements during water injection, (b) PPT measurements during injection of sodium percarbonate solution for TEST 2

The pressure measurements in TEST 2 during injection of sodium percarbonate solution were consistent with the decreasing trend in the flow measurements presented in
Figure 5-27 (b). Performance of PPT 4 and PPT 5 were not good during injection of solution due to the presence of gas bubbles in or around the pressure transducers.

In general, flow and pressure measurements in TEST 2, were similar to those recorded in TEST 1.

5.2.2.2 Transport of Chemical Solution – TEST 2

The electrical conductivity measurements of TEST 2 are presented in Figure 5-29. Similar to TEST 1, electrical conductivity values peaked as the solution arrived at a probe location. In TEST 2, the peak values of the conductivity were 1.5 to 2.4 mS/cm lower than the values in TEST 1 (2.8 to 3.5 mS/cm). The lower peak values in TEST 2 are expected because of lower concentration of the solution injected.

Figure 5-29 shows that the solution arrived at probes EC1 through EC9 except EC8. Electrical conductivity measured at the location of EC8 did not increase during injection of the solution. Based on the electrical conductivity data, it was concluded that the boundary of the zone of influence of concentration of solution in TEST 2 was somewhere between probes EC9 (~20 away from injection) and EC8 (~25 cm away from injection). The radius of the zone of influence of concentration of solution was determined to be around 20 cm.
Figure 5-29 Locations of electrical conductivity probes (b) Electrical conductivity values measured at 12 probe locations during 13 minute injection of solution for TEST 2

The results of the Brix probe confirmed the arrival of 0.5% concentration (design concentration in TEST 2) at the locations of probes EC1 through EC7 and EC9.
Table 5-3  Brix probe measurements of sodium percarbonate concentrations – TEST 2

<table>
<thead>
<tr>
<th>EC Probe</th>
<th>Distance from injection, cm</th>
<th>Brix Probe reading</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC1</td>
<td>0</td>
<td>0.5%</td>
</tr>
<tr>
<td>EC2</td>
<td>0</td>
<td>0.5%</td>
</tr>
<tr>
<td>EC3</td>
<td>10</td>
<td>0.4%</td>
</tr>
<tr>
<td>EC5</td>
<td>10</td>
<td>0.5%</td>
</tr>
<tr>
<td>EC6</td>
<td>10</td>
<td>0.4%</td>
</tr>
<tr>
<td>EC7</td>
<td>15</td>
<td>0.5%</td>
</tr>
<tr>
<td>EC9</td>
<td>20</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

5.2.2.2.3 Degree of Saturation – TEST 2

Measurements of electric conductivity were made in TEST 2 for 16 hours to identify the final zone of partial saturation and as to estimate degree of saturation (Figure 5-30). The long duration of recording was necessary since the rate of the gas generation reaction is slower for 0.5% concentration than for 1% concentration, as was discussed in Section 4.2.1 of Chapter 4.

Figure 5-30 shows that the arrival of the solution at probe EC8 was after the 13 minutes of injection. The solution arrived at EC8 about 2 hours after the start of the test by diffusion. The solution that arrived at probe EC8 must have contained some level of hydrogen peroxide because the reaction did not end after 2 hours for 0.5% concentration. The decreasing trend in electrical conductivity values at EC8 confirmed the gas generation at this location.
Figure 5-30 Electrical conductivity values measured during injection and gas generation - TEST 2

Figure 5-31 presents the calculated degree of saturation as a function of time at each probe location using the electrical conductivity measurements. The degree of saturation values were estimated to be in the range of 54 to 77%. The average of degree of saturation values obtained from the 9 probe measurements was about 69% in TEST 2, and was higher than that of in TEST 1, 65%. The difference is within the accuracy of the electrical conductivity measurements therefore it is not definite to relate this difference to the lower concentration used in TEST 2. The average value of degree of saturation from probe measurements (69%) was again compared with the batch experiment conducted with concentration of 0.5% which was (73%). The agreement between these two values was reasonable.

The final values of degree of saturation obtained by the probes are superimposed on the photo of the specimen of TEST 2 in Figure 5-32.
Figure 5-31 Results for degree of saturation at probes EC1 through EC9 – TEST 2

Figure 5-32 Picture of partially saturated sand specimen – TEST 2
Based on the visual observations, a line which designates the zone of partial saturation was drawn in Figure 5-32. The zone of partial saturation extends to the probe EC8 similar to electrical conductivity probe measurements. Therefore, the radius of the zone of partial saturation was estimated to be approximately 25 cm based on electric conductivity measurements and on visual observation. This is slightly smaller than the 30 cm radius observed in TEST 2 because the more pronounced reduction in the inflow of solution was measured during injection of solution in TEST 2 than that of in TEST 1.

Micro images were also taken from selected locations in TEST 2, identifying gas bubbles, as shown in Figure 5-33.

**TEST 2**

![Figure 5-33 Digital images of fully and partially saturated specimens showing gas bubbles for TEST 2](image)

The measurements of outflow from TEST 2 during gas generation are presented in Figure 5-34. The average degree of saturation in the zone of partial saturation was calculated using outflow measurements with the same logic as was presented for TEST 1 in Section 5.2.2.1.3.
Average degree of saturation

\( S_{\text{AVE}} \) in the zone of partial saturation using outflow measurements:

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

\( e = 0.72 \) and \( n = 0.42 \)

\( V_t = 67387 \text{ cm}^3 \)

\( (V_v) \text{ for entire specimen} = n (V_v) = 0.42 \times 67387 = 28209 \text{ cm}^3 \)

\( (V_v) \text{ for partially saturated zone} = (0.40 \text{ to } 0.45) \times (V_v) \text{ for entire specimen} \)

\[ 0.40 \times 28209 = 11283 \text{ cm}^3 \]

\[ 0.45 \times 28209 = 12694 \text{ cm}^3 \]

\( (S_{\text{AVE}}) = (V_v - V_{\text{bubble}}) / V_v \)

for 40% zone of partial saturation \( (S_{\text{AVE}}) = (11283-1483)/11283 = 0.86 = 86\% \)

for 45% zone of partial saturation \( (S_{\text{AVE}}) = (12694-1483)/12694= 0.88 = 88\% \)

The percent volume of the partially saturated zone in TEST 2 was assumed to be in the range of 40 to 45% which is approximately 20% smaller than TEST 1. The average degree of saturation calculated using the outflow measurements of TEST 2 was in the range of 86 to 88%. This average degree of saturation from outflow measurements was quite high compared to the average degree of saturation estimated using electrical conductivity measurements which was 69% as well as the degree of saturation value obtained from batch experiment with 0.5% concentration which was 73%. The underestimation of the collected outflow was more pronounced in TEST 2. This was attributed to the smaller volume of gas bubbles (due to lower injection concentration) and hence smaller amount of outflow. As the amount of pore fluid to be collected in the outflow bucket got smaller, the inaccuracy in the measurements became more pronounced. Considering the uncertainties involved in
both methods of estimation of degree of saturation (probes and volume calculations), it was concluded that the degree of saturation within the partially saturated zone was about 70% in TEST 2.

Figure 5-34 Outflow measured during gas bubble generation - TEST 2
5.3 SUTRA-Bubble Simulations of Glass Tank Experiments

This section presents the SUTRA-Bubble simulations performed for glass tank experiments (TEST 1 and TEST 2) that were presented in Section 5.2. Again, the purpose of these simulations was to validate SUTRA-Bubble. The preparation of the input files for the simulation was the same for both tests except the boundary condition for injection. The input data included; size of the mesh, soil parameters such as porosity and saturated permeability, and boundary conditions for injection. The steps involved in the SUTRA-Bubble comparisons made with the experimental results for validation are outlined in Figure 5-35.

As shown in Figure 5-35, the dimensions of the specimen, locations of the instruments and porosity values measured were used to create the mesh geometry for both tests. In addition, the saturated permeability was needed in the SUTRA-Bubble simulation. Since permeability is an important parameter, instead of using typical values for Ottawa sand obtained through 1D flow experiments, it was back-calculated for the sand specimen prepared in the glass tank. SUTRA-Bubble was run for glass tank experiments simulating clean water flow with the inflow measured from the experiment as input at the injection tip. The value of the permeability of the saturated specimen was varied until the pressures at the injection tip matched with the experiment results. The permeability value was then used in subsequent SUTRA-Bubble simulations.

For validation of SUTRA-Bubble, three sets of results from the outputs of the simulations were compared with the corresponding measured data from the experiments.
Sets of results used:

1. Flow and pressure during injection
2. Transport of solution
3. Degree of saturation

**SUTRA-Bubble Validation**

**Experiment**
- Determine:
  - Exact specimen height
  - Exact location of instruments,
  - Porosity
- Inject Clean Water
  - Measure:
    - Inflow of de-aired water
    - $\Delta H(TIP)$
- Inject Sodium Percarbonate Solution
  - Injection parameters
    - Pressure head
    - Concentration of Solution
    - Duration of Injection
  - Measurements
    - Inflow and pressure during injection
    - Outflow during and after injection
    - Electrical conductivity in soil
    - Concentration of solution in soil

**Simulation**
- Create Mesh geometry for sand specimen with boundary conditions including injection tube
  (Same for both tests)
- Run SUTRA-Bubble simulation of water injection using measured inflow as an input
  Back-figure saturated hydraulic conductivity, $k_{sat}$ by matching predicted and measured $\Delta H(TIP)$
- SUTRA-Bubble Simulation of Injection of Solution
  - Input parameters
    - $k_{sat}$
    - Concentration of solution
    - Duration of injection
    - Inflow during injection (from experiment)
  - Outputs
    - Pressure during injection
    - Outflow
    - Concentration of solute in soil
    - Degree of saturation
    - Partial saturation zone

**SUTRA-Bubble Validation**
- Compare Experiment and SUTRA-Bubble;
  - Flow and pressure
  - Transport of chemical solution
  - Degree of Saturation

Figure 5-35 Steps for validation of SUTRA-Bubble predictions
5.3.1 Preparation of SUTRA-Bubble Simulation

The preparation of the SUTRA-Bubble simulation included:

- Preparation of mesh structure
- Assignment of boundary and initial conditions for injection of clean water or solution
- Assignment of soil parameters and simulation controls

Preparation of mesh structure

Argus ONE with a plug in extension of SutraGUI was the software used as the graphical user interface for preparing input files for SUTRA simulations. A 3D mesh for the sand specimen in the glass tank was prepared to run SUTRA-Bubble simulations for TEST 1 and TEST 2. The mesh geometry was the same for both tests.

Figure 5-36 shows the image of the mesh prepared both in 3D and elevation views along with pictures of the specimen in the glass tank. In order to create the 3D mesh for the sand specimen, the plan view of the sand specimen with dimensions of 91 cm in length and 13.5 cm in width was extruded in elevation to the measured height of the sand specimen which was 55 cm for both tests. The mesh was divided into 12 layers in elevation in order to be able to identify locations of the nodes for injection as well as the nodes corresponding to the locations of electrical conductivity probes and pore pressure transducers. Dividing into different layers allowed the assignment of the boundary condition for injection (source of flow/specified pressure) at injection nodes and requesting for observation outputs at nodes corresponding to instrument locations. The injection nodes can be seen in Figure 5-36 at a depth of 25 cm. These observation nodes at the instrument locations gave the outputs of pressure and degree of saturation with time. At the top of the specimen, a
boundary condition of specified pressure of zero was assigned to simulate the free water surface.

The soil elements in the 3D mesh were aligned hexahedral elements with eight corners. The size of the elements were identical for the whole mesh with a width of 0.5 cm. The fine discretization of the mesh in elevation can be seen in Figure 5-36 (b).

**Figure 5-36 SUTRA-Bubble mesh for Glass Tank experiment set up**
(a) 3-D view
(b) Elevation view

Figure 5-36 SUTRA-Bubble mesh for Glass Tank experiment set up (a) 3-D view of the mesh (b) elevation view of the mesh
The entire mesh was created as soil elements even at the location of the injection tube. Since the soil elements above the injection nodes cannot be part of the flow model, in other words there should not be any flow going into the elements right above the injection nodes, for these elements a very low permeability (1e-30 m²) was assigned (Figure 5-37).

![Soil elements at the injection tube location](image)

Figure 5-37 Soil elements at the injection tube location

Figure 5-38 includes the images from the mesh showing the permeability values assigned in the mesh for the regular soil elements of sand and impermeable “soil” elements representing the injection tube. Figure 5-38 also includes the velocity vectors both in elevation and plan view, demonstrating no flow in the impermeable zone simulating the injection tube.

Assignment of boundary and initial conditions for injection of clean water or solution

Rate of inflow measured during an experimental test was assigned as the source of flow in order to simulate the injection process of either clean water or solution. The rate of inflow was constant for clean water injection. Therefore, a constant rate of inflow was assigned for the clean water simulations. However, the flow rate was decreasing during
injection of solution due to gas bubbles trapped at the tip of the injection tube. Therefore, time-dependent boundary condition option was used to prepare the proper input data for injection of solution.

The discrete measurement at certain times during the injection process both in TEST 1 and TEST 2 were used to prepare a separate file (".bcs" file) for time-dependent boundary condition in SUTRA-Bubble simulations. In that "bcs" file, the variable flow rate at each time step was listed along with the corresponding design concentration for each
injection node. Separate files were prepared for TEST 1 and TEST 2 since the flow rate measurements were different.

It is noted that the solute concentration in SUTRA-Bubble, $C$ was the concentration of hydrogen peroxide, $\text{C}_\text{H}_2\text{O}_2$. Equation (3-41) presented in Section 3.3.1 in Chapter 3 related $C$ to the design concentration of sodium percarbonate, $C_{\text{SPC}}$ and efficiency coefficient, $E_f$. The efficiency parameter, $E_f = 76\%$ as was described in Section 4.2.2 of Chapter 4. Input concentration of solute, $C$ in SUTRA-Bubble was then calculated by Equation (3-41) using $C_{\text{SPC}}$ and $E_f$. Table 5-4 shows the input concentration of solute, $C$ assigned at the injection nodes corresponding to the design concentration of sodium percarbonate, $C_{\text{SPC}}$ for both TEST 1 and TEST 2.

Table 5-4 Input concentration values used in SUTRA-Bubble simulation

<table>
<thead>
<tr>
<th>Design concentration of sodium percarbonate $C_{\text{SPC}}$ (Measured)</th>
<th>SUTRA-Bubble input concentration $C = (\text{C}_\text{H}_2\text{O}_2)$ Equation (3-41)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEST 1 (kg/kg) 0.01 (1%)</td>
<td>0.002468</td>
</tr>
<tr>
<td>TEST 2 (kg/kg) 0.005 (0.5%)</td>
<td>0.001234</td>
</tr>
</tbody>
</table>

Finally, the free water surface was simulated by assigning specified zero pressure at the nodes on top of the mesh. The nodes at the two sides and bottom of the specimen with no assignment were automatically assumed to be impermeable representing the walls of the glass tank.
Initial conditions were assigned as hydrostatic pressures since the free water surface was at the top of the sand. The initial conditions for concentration was zero everywhere within the mesh.

**Assignment of soil parameters and simulation controls**

The rest of the input data were porosity, dispersivity, density coefficient for variable density flow, rate parameter for reaction, and all temporal and numerical controls that were all described in Section 3.6.

The list of the input parameters used in SUTRA-Bubble simulation for both TEST 1 and TEST 2 is presented in Table 5-5.
Table 5-5 Summary of parameters used in SUTRA-Bubble simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>TEST 1</th>
<th>TEST 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size of model</td>
<td>91 cm (L) x 13.5 cm (W)</td>
<td>91 cm (L) x 13.5 cm (W)</td>
</tr>
<tr>
<td>Specimen height</td>
<td>55 cm</td>
<td>55 cm</td>
</tr>
<tr>
<td>Depth of Injection tip</td>
<td>25.5 cm</td>
<td>25.5 cm</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.41</td>
<td>0.42</td>
</tr>
<tr>
<td>Average Saturated Permeability</td>
<td>1.5 E-10 m² *</td>
<td>1.75 E-10 m² *</td>
</tr>
<tr>
<td>Dispersivity (Long. &amp; Trans.)</td>
<td>1E-3 m</td>
<td>1E-3 m</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>1E-9 m²/s</td>
<td>1E-9 m²/s</td>
</tr>
<tr>
<td>Coefficient of density change ( \frac{\partial \rho}{\partial C} )</td>
<td>4052 (kg/m³)</td>
<td>4052 (kg/m³)</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>Hydrostatic pressure</td>
<td>Hydrostatic pressure</td>
</tr>
<tr>
<td>Initial concentration</td>
<td>0 (kg/kg)</td>
<td>0 (kg/kg)</td>
</tr>
<tr>
<td>Actual concentration of H₂O₂ solution ( C_{H₂O₂} )</td>
<td>0.002468 (kg/kg)</td>
<td>0.001234 (kg/kg)</td>
</tr>
<tr>
<td>Duration of injection</td>
<td>13 minutes</td>
<td>13 minutes</td>
</tr>
<tr>
<td>Total duration of the model</td>
<td>360 minutes</td>
<td>600 minutes</td>
</tr>
<tr>
<td>Time increment</td>
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<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>
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<tr>
<td>Mesh size</td>
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<td>0.5 cm (hexahedral)</td>
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<td>571872</td>
</tr>
<tr>
<td>Number of elements</td>
<td>543510</td>
<td>543510</td>
</tr>
<tr>
<td>Solver for pressure</td>
<td>Iterative – GMRES</td>
<td>Iterative – GMRES</td>
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<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>

* Back-calculated from matching measured & SUTRA-Bubble predicted pressures from clean water runs (refer to Section 5.3.2)
5.3.2 Back-calculation of Saturated Permeability of Sand Specimen

This section presents how the saturated permeability for the sand specimens of TEST 1 and TEST 2 were back-figured by matching SUTRA-Bubble predicted pressures at injection nodes with measured pressures at the tip of the injection tube. As mentioned earlier, measured data of inflow of clean water in TEST 1 and TEST 2 were assigned as input for injection. The pressure outputs of the simulation at injection nodes were compared with the applied pressure at the injection tip. The permeability value (same in both horizontal and vertical directions) that led to a match of the predicted and the measured pressures was determined as the saturated permeability of the specimen. It is understood that the horizontal and vertical permeability values probably are different in the sand specimens primarily due to the deposition by wet pluviation. The back-calculated permeability can be considered as an average permeability for the entire specimen that yields good predictions by SUTRA-Bubble. Therefore, it is reasonable to assume that its use in subsequent simulations will also yield reasonable predictions.

Figure 5-39 (a) and (b) show the input flow of clean water and predicted pressures by SUTRA-Bubble with the permeability values converged for TEST 1 and TEST 2, respectively. The back-figured values of the saturated permeability were 1.5 E-10 m² for TEST 1 and 1.75 E-10 m² for TEST 2.
Figure 5-39 Input flow of clean water and SUTRA-Bubble prediction at injection nodes  
(a) TEST 1 (b) TEST 2

In addition, model-predicted pressures at the locations of the pore pressure 
transducers were compared with the experimentally measured pressures as shown in Figure 
5-40. The predicted pressures at PPT 1 and PPT 2, which were very close to the injection 
tube matched well with the measured values. However, the match for the PPT’s 3, 4, and 
5 was not as good. This difference can be attributed to the use of the same permeability 
values in horizontal and vertical directions. A larger permeability in the horizontal 
direction than the average permeability used could lead to smaller head losses and thus 
higher pressure heads.
Figure 5-40 (a) Locations for pore pressure transducers; Comparison of predicted and measured pressures (b) for TEST 1 (c) for TEST 2
5.3.3 SUTRA-Bubble Outputs

SUTRA-Bubble simulation outputs of concentration of solution (Hydrogen peroxide) and degree of saturation for TEST 1 and TEST 2 are presented in this section.

The images of the outputs were prepared by Model Viewer program and presented in 3-D view and along three different sections. Locations of Sections A-A, B-B, and C-C are shown in Figure 5-41.

![Figure 5-41 Section A-A, B-B, and C-C of the SUTRA-Bubble mesh](image)

5.3.3.1 Outputs – TEST 1

The output of concentration from SUTRA-Bubble simulation for TEST 1 at 15 minutes (right after injection was completed) are presented in Figure 5-42. The concentration outputs show the zone of influence of the transport of the solution achieved at the end of injection.
Figure 5-42 Concentration outputs of SUTRA-Bubble simulation for TEST 1 at 15 minutes after injection (a) 3-D view (b) Section C-C (c) Section A-A (d) Section B-B
The 3D view of the outputs were cropped in both longitudinal and transverse directions in order to show the outputs around the injection tube. The concentration contours right above the injection nodes representing the injection tube were not relevant numbers because the tube was modeled as an impermeable sand. The zone of influence was almost circular and symmetric around the injection tube, as expected. The results along Section B-B (Figure 5-42 (d)) show the almost uniform concentration of solution on the narrow side of the glass tank. The tank was designed to be narrow in order to make the glass sides of the tank representative of the center line of the tank where all the instruments were. The uniform concentration output along Section B-B shows that the results along the sides were the same as along the center line. This was also confirmed by the visual observations from the glass sides of the tank. It is observed from the concentration output along Section A-A (Figure 5-42 (c)) that the circular zone of influence was dominated by the full concentration of injection (equivalent to the design concentration sodium percarbonate of 1%). This showed that the transport of the concentration of solution was dominated by the flow due to hydraulic gradient during injection. The mixing effect of fluid velocity on concentration of solution (dispersion) as well as the diffusion of the concentration of the solution was insignificant during injection. The solution was transported ~27 cm away from the injection tube in the horizontal direction and ~ 24 cm away in vertical direction, during the 13-minute injection, as shown along Section A-A and Section C-C.

The results of degree of saturation obtained from SUTRA-Bubble simulation for TEST 1, at the end of gas generation (6 hours after injection) are presented in Figure 5-43. Section A-A shows that the partially saturated zone extended ~31 cm away from the
injection tube in the horizontal direction and ~ 27 cm away from the injection tube in the vertical direction, which were both larger than the zone of influence for transport of the solution during injection. The 4 cm difference in horizontal direction can be attributed to possible diffusion of the solution with concentration gradient which SUTRA-Bubble accounts for. The 3 cm difference in vertical direction can be due to both diffusion of solution and flow due to gradient in fluid density. It is also recognized that the degree of saturation contours appear to spread in the horizontal direction more than vertical near the bottom impermeable boundary. This boundary effects can also be observed in Figure 5-43 (c) where saturation outputs along Section B-B are presented. Plot of degree of saturation along section D-D cut from a location very close to the bottom boundary is presented in Figure 5-44, and shows the effect of the side boundaries on the shape of the saturation contours.

Values of degree of saturation obtained at the end of 6 hours were mostly in the range of 0.50 to 0.65 (50 to 65%) in the partial saturation zone.
Figure 5-43 Degree of saturation outputs of SUTRA-Bubble simulation for TEST 1 (a) Section C-C (b) Section A-A (c) Section B-B

Figure 5-44 Degree of saturation output of SUTRA-Bubble simulation for TEST 1 for Section D-D
5.3.3.2 Outputs – TEST 2

SUTRA-Bubble simulation was also performed for TEST 2, where the design concentration of sodium percarbonate, \((C_{spc})_{design}\) was 0.5%. The outputs of concentration from SUTRA-Bubble simulation for TEST 2 at 15 minutes are presented in Figure 5-45. The outputs were similar to TEST 1, with different initial value of concentration of hydrogen peroxide that is calculated from 0.5% concentration of sodium percarbonate injection in TEST 2. Also, the predicted zone of influence was slightly smaller than TEST 1. In TEST 2, the solution was transported \(\sim24\) cm away from the injection tube in the horizontal direction and \(\sim22\) cm away in the vertical direction, during the 13-minute injection. This distance is shorter than that of in TEST 1 because the more pronounced reduction in the inflow of solution was measured during injection of solution in TEST 2 than that of in TEST 1.
Figure 5-45 Concentration outputs of SUTRA-Bubble simulation for TEST 2 at 15 minutes after injection (a) 3-D view (b) Section A-A (c) Section B-B
The results for degree of saturation from the simulation of TEST 2 are presented in Figure 5-46. The shape of the contours is similar to TEST 1, whereas the final degree of saturation values are in the range of 0.70 to 0.80 (70 to 80%); higher than for TEST 1 (50 to 65%) because of lower concentration of the injected solution.

The partial saturation zone in TEST 2 extended ~28 cm away from the injection tube in the horizontal direction and ~25 cm in the vertical direction, which were both larger than the zone of influence for transport of the solution (contours of concentration) as shown in Figure 5-46 (b). The 4 cm difference in the zone of degree of saturation and zone of concentration in the horizontal direction is attributed to diffusion, and the 3 cm difference in the vertical direction can be attributed to both diffusion of solution and flow due to
gradient in fluid density. The zone of partial saturation for TEST 2 (28 cm by 25 cm) was predicted to be slightly smaller than TEST 1 (31 cm by 27 cm) because of the more pronounced reduction in the inflow of solution measured in TEST 2 than that of in TEST 1.

### 5.4 Comparison of SUTRA-Bubble Predictions with Experimental Results

Predictions from the SUTRA-Bubble simulations of TEST 1 and TEST 2 experiments were compared with the experimental data presented in Section 5.2. The comparison was made again using 3 sets of results:

1. Flow and pressure during injection
2. Transport of chemical solution
3. Degree of saturation

This section presents the comparisons for TEST 1 followed by those made for TEST 2.

#### 5.4.1 Comparisons for TEST 1

#### 5.4.1.1 Flow and Pressure during Injection – TEST 1

The measured inflow during injection in the experiment of TEST 1 was used as the input parameter for injection in SUTRA-Bubble simulations in order to properly simulate the actual condition in the experiment. Figure 5-47 shows the inflow assigned in the simulation of TEST 1.
Figure 5-47 Inflow assigned for 13 minutes in SUTRA-Bubble simulation of TEST 1

SUTRA-Bubble outputs for both inflow and outflow of the solution during injection together with the experimental measurements are presented in Figure 5-48. Figure shows that the input flow was properly assigned and the predicted outflow during injection matches well with experimental measurements. The predicted and measured outflow of solution was almost the same as the inflow of solution. This indicates that the change in degree of saturation in the sand specimen was insignificant during the 13-minutes of injection of solution. This also confirms the assumption made in the calculation of the degree of saturation using electrical conductivity that gas generation during the short duration of injection was negligible.
Figure 5-48 Inflow and outflow values computed by SUTRA-Bubble for TEST 1 compared with measured data

Further discussions on outflow due to gas generation during the 6 hours after injection are included in Section 5.4.1.3.

In addition to flow, predictions of pore water pressure during injection were compared with the pressures measured by the pore pressure transducers, as shown in Figure 5-49. The predicted pressures during injection of solution were slightly lower than the measured pressures, which is similar to the case of clean water injection (Figure 5-40). This discrepancy between the predicted and measured pressures was essentially attributed to the isotropic permeability approximation.
Figure 5-49 Comparison for predicted and measured pressures for TEST 1

(a)

(b)

(c)

Figure 5-49 Comparison for predicted and measured pressures for TEST 1
It was also observed that the drop in measured pressures within the first 3 minutes were not predicted by the simulation. Predicted pressures strictly followed the trend in the rate of inflow. Possible discrepancy between the measured inflow and pressures led to the discrepancy between the predicted and measured pressures. Overall, the SUTRA-Bubble predictions of pore water pressure agree with experimentally measured results.

5.4.1.2 Transport of Chemical Solution – TEST 1

In Figure 5-50 the spatial distribution of the predicted concentration of solute (hydrogen peroxide) for TEST 1 were plotted together with the location of each electric conductivity probe.

![Figure 5-50 Concentration output of SUTRA-Bubble for TEST 1 with superimposed locations of electric conductivity probes](image)

Predicted concentrations show that the contour for maximum concentration of hydrogen peroxide (0.00247 kg/kg) which was equivalent to the concentration of sodium percarbonate in TEST 1 (1% by weight), reached just about to the probe EC 8. Figure 5-50 also shows that the solution did not arrive at the location of the probes EC10 through EC12.
The solution traveled about 25 cm away from the injection tube (about 27 cm in the horizontal direction and 24 cm in the vertical direction) during injection. The experimental data on concentration of solution also demonstrated that the boundary for the zone of influence of solution was in between probes EC8 (~25 cm away from injection) and EC11 (~30 cm away).

In addition, predicted and measured concentration values, which represented the transport of the solution to each probe location as a function of time were compared. The transport of the chemical was measured using the electrical conductivity probes. The change in electrical conductivity with time represented the change in concentration at the probe location, which is referred to as the concentration breakthrough curve at that location. These breakthrough curves at each probe location during injection were compared with the predicted concentration as a function of time at those locations. However, since the units of the predicted curves (kg/kg) are different from those measured by the probes (mS/cm) the curves were normalized with their peak values representing the maximum concentration at that location. These normalized breakthrough curves at each probe location are presented in Figure 5-51 and Figure 5-52.

All the measured breakthrough curves shown in Figure 5-51 and Figure 5-52 indicated that advective transport, which is the transport of solution with the hydraulic gradient, was quite dominant during injection. Therefore, the dispersivity value, which represents the mixing effect of fluid velocity on the transport of solution, was selected to be the smallest possible that can be used for the mesh size. The dispersivity value used in the simulations was $1 \times 10^{-3}$ m, which is in the range of typical values for clean sands ($1 \times 10^{-3}$ to $1 \times 10^{-1}$ m from Gillham and Cherry, 1982). Both figures show that the predicted and
measured values compare well at each probe location in regards to arrival time of the peak concentration. The arrival time of the solution at each probe location was consistent with the distances of the probes from the injection tip. Figure 5-51 (b) shows immediate arrival of the maximum concentration at probes EC1 and EC2, because they were very close to the injection tip. At probes EC1 and EC2, during the early stage of the decay of hydrogen peroxide solution, the measured and the predicted curves are slightly different. The decrease from the peak representing gas bubble generation for the measured data is faster than that of the predicted values at these locations. This is not observed in any other probe location. Probes EC1 and EC2 were very close to the tip of the injection tube where the soil deposition around the probe may not have been representative of the typical soil density in the specimen. In Figure 5-51 (c), the arrival times at 2 minutes at probes EC3, EC5, and EC6 (10 cm away from injection) from the experimental data and from the simulated predictions agree very well. The arrival of solution at probe EC7, which was 15 cm away from the injection tip, was measured as 3 minutes and predicted as 4 minutes after injection as shown in Figure 5-52 (a). This is again a good agreement. The arrival of solution at probes EC4 and EC9, which were approximately 20 cm away from injection, were measured to be approximately 6 minutes and the predicted was 8 minutes (Figure 5-52 (b)). Finally, Figure 5-52 (c) shows that at probe EC8 the measured arrival time was 12 minutes and the predicted time was approximately 14 minutes.

In summary, the predicted breakthrough curves by SUTRA-Bubble matched well with the measured curves. The arrival times of the solution to the location of the probes observed in the experiment of TEST 1 agreed well with those predicted by SUTRA-Bubble.
Figure 5-51 (a) Locations of electrical conductivity probes (b) breakthrough curve at probes EC1 and EC2 (c) breakthrough curve at probes EC3, EC5, and EC6
Figure 5-52 (a) Breakthrough curve at probe EC7 (b) breakthrough curve at probes EC4 and EC9 (c) breakthrough curve at probe EC8
5.4.1.3 Degree of Saturation – TEST 1

The results of degree of saturation predicted by SUTRA-Bubble for TEST 1 were compared with those from the glass tank experiment. The spatial distribution of the predicted degree of saturation for TEST 1 are plotted together with the locations of each electric conductivity probe in Figure 5-53.

Figure 5-53 shows that the predicted zone of partial saturation extends to probe EC11. The predicted zone of partial saturation does not reach probes EC10 and EC12. The maximum distance of the predicted partial saturation zone is 31 cm from the injection tube in the horizontal direction, and 27 cm in the vertical direction, as shown in Figure 5-53. Similar observations were made on the extent of the partial saturation zone from the experimental measurement in TEST 1 (30 cm away from injection tube). Therefore, it can be concluded that SUTRA-Bubble prediction of the size of the zone of partial saturation is in good
agreement with the experimental results. The prediction of the zone of partial saturation relates to the proper assignment of inflow of solution.

In addition to the size of zone of partial saturation, values of predicted degree of saturation at each probe location were compared with those obtained from the experimental measurements. Figure 5-54 shows the degree of saturation predictions of SUTRA-Bubble plotted for 6 hours together with the experimental results. The predicted degree of saturation at all probe locations decreases generally exponentially, consistent with the exponential gas generation model implemented in SUTRA-Bubble. The predicted degree of saturation in general matches well with the experimental results. The measured data show that there was no significant change in the degree of saturation after 2 hours, whereas SUTRA-Bubble predicted further reduction in degree of saturation after 2 hours. For this reason, at the end of the reaction, predicted degree of saturation values in TEST 1 is slightly lower than in the measured data. This may indicate that the assumed exponential generation of gas bubble may not be a perfect fit of the real data, but is a mathematically convenient formulation that yields generally good results.
The degree of saturation predicted by SUTRA-Bubble for all probe locations ranged between 55% and 58%. The average degree of saturation of the predicted values at
the 9 probe locations was 57%. The degrees of saturation calculated from the electrical conductivity measurements were in the range of 59% to 73%. The average value of the degree of saturation values measured by 9 electrical conductivity probes was 65%, as was presented in Section 5.2.2.1.3. The experimental results probably included the effect of local heterogeneities in the specimen, a factor that is not accounted for by SUTRA-Bubble. Based on these comparisons it was concluded that SUTRA-Bubble predictions of degree of saturation for TEST 1 were satisfactory when compared with the experimental measurements.

SUTRA-Bubble predictions of outflow during gas generation is compared with the measured outflow data, in Figure 5-55. The outflow predicted by SUTRA-Bubble for the first 2 hours agrees well with the measured values, with only a small difference between the two outflows. By the end of the reaction (6 hours), the SUTRA-Bubble prediction for outflow was greater than the experimentally measured values. This discrepancy is attributed to the inability to collect efficiently the small quantity of outflow from the surface of the specimen in the glass tank, as was also described in Section 5.2.2.1.3. Therefore, SUTRA-Bubble predictions of outflow are considered to be reasonable.

![Figure 5-55 Comparison of predicted and measured outflow of solution for TEST 1](image-url)
5.4.2 Comparison for TEST 2

Similar to TEST 1, predictions from SUTRA-Bubble simulation performed for TEST 2 were compared with experimental measurements. The comparisons were made in the same format used for TEST 1 above. The design concentration for TEST 2 was 0.5% compared with 1% for TEST 1.

5.4.2.1 Flow and Pressure during Injection – TEST 2

Measured inflow data was used as an input for SUTRA-Bubble simulation of TEST 2. The inflow data measured at every minute was assigned as shown in Figure 5-56.

SUTRA-Bubble outputs for both inflow and outflow of the solution together with the experimental measurements are presented in Figure 5-57. The reduction in the inflow of solution and thus corresponding drop in pressures were properly simulated.

Figure 5-56 Inflow assigned for 13 minutes in SUTRA-Bubble simulation of TEST 2
Figure 5-57  Inflow and outflow values computed by SUTRA-Bubble for TEST 2 compared with measured data

Figure 5-58 shows the predicted and measured pressures for all the PPT’s located in the specimen except PPT 5. PPT 5 was not included in the comparison since it malfunctioned during injection of solution. The locations of the instruments were presented earlier in Figure 5-49. The predictions of the pressures at PPT 1 and PPT 2 compared with the measured data were quite good. The comparisons of the pressures at PPT 3 and PPT 4 were reasonably good. The measured pressures at PPT 4 were not very reliable because they eventually it dropped below hydrostatic at that location.
5.4.2.2 Transport of Chemical Solution – TEST 2

The spatial distribution of concentration predicted by SUTRA-Bubble for TEST 2 is plotted together with the locations of each electric conductivity probe in Figure 5-59.
Since the flow was slower in TEST 2, SUTRA-Bubble concentration outputs show that the maximum concentration (0.00123 kg/kg), which is equivalent to 0.5%, reached probe EC9 but not EC8. The zone of the experimental data on concentration of solution also demonstrated that the boundary for the zone of influence of concentration of solution was in between probes EC9 and EC8 and the radius of the zone was determined to be 20 cm.

The transport of the solution was also detected through the electrical conductivity measurements using breakthrough curves. The details of the preparation of breakthrough curves were explained in the discussion of the results for TEST 1. The breakthrough curves for TEST 2 at all probe locations are presented in Figure 5-60. In general, the predictions of SUTRA-Bubble were in good agreement with the probe measurements.
Figure 5-60 Breakthrough curves at probes (a) EC1 and EC2 (b) EC3, EC5, and EC6 (c) EC7 and (d) EC4 and EC9 - TEST 2
Probe EC8 showed that during injection in TEST 2, the solution did not arrive at probe EC8 but after injection the solution was transported through diffusion. In Figure 5-61, the comparison of the breakthrough curves at probe EC8 is presented. The late arrival of the solution at probe EC8 was due to diffusion of solution after injection. The breakthrough of concentration due to diffusion was very slow. These were observed both from the predicted and the measured curves. However, predicted arrival time of solution was earlier than the arrival time measured by the probes. It is noted that the travel distance for concentration of solution due to diffusion is very small (in the order of 3-4 cm) due to its slow rate compared to hydraulic gradient. In this case, the predictions of arrival times were very sensitive to precise selection of the probe locations in the mesh, where slight change in location can lead to substantial differences in arrival times.

![Arrival of Solution - EC8](image)

Figure 5-61 Breakthrough curve at probe EC8 – TEST 2

**5.4.2.3 Degree of Saturation – TEST 2**

The predicted degree of saturation from SUTRA-Bubble for TEST 2 was compared with the conductivity probe results. The spatial distribution of degree of saturation predictions of SUTRA-Bubble are presented with the probe locations in Figure 5-62. It is noted that the partial saturation zone extends to the location of probe EC8. The predicted
distance of the partial saturation zone away from the injection tube was \(~28\) cm in horizontal and \(~25\) cm in vertical directions. The experimental data showed that the zone of partial saturation extended approximately \(25\) cm away from the injection tube. The size of the partial saturation in TEST 2 obtained through SUTRA-Bubble prediction and experiment measurements were in good agreement similar to TEST 1.

**Figure 5-62** Degree of saturation output of SUTRA-Bubble for TEST 2 with superimposed locations of electric conductivity probes

Figure 5-63 presents the predicted degree of saturation in TEST 2 plotted together with the measured degree of saturation for 10 hours. Similar to TEST 1 the degree of saturation predicted by SUTRA-Bubble at all probe locations followed approximate exponentially decreasing function. In general, the comparison of predicted and measured degree of saturation values were satisfactory considering the sources of experimental inaccuracies involved. The comparison was not as good at probe EC8 since it was very close to the boundary of the partial saturation zone. The final degrees of saturation
predicted by SUTRA-Bubble for all the probe locations were in the range of 75% and 78% (average value of 76%), and agreed well with the estimated values from measured data which were in the range of 54% to 77% (average value of 69%).

Figure 5-63  Comparison of predicted and measured degree of saturation for TEST 2
Finally, the comparison between the predicted and measured outflow for TEST 2 are presented in Figure 5-64. Similar to TEST 1, the predicted values of outflow were higher than those measured, which was determined to be underestimated due to inability to collect efficiently the small quantity of outflow from the surface of the specimen in the glass tank. The difference between the predicted and measured data is more pronounced in TEST 2. This was attributed to the smaller volume of outflow compared to those measured in TEST 1 due to lower injection concentration, which led to more inaccuracies in outflow measurements.

![Figure 5-64 Comparison of predicted and measured outflow of solution for TEST 2](image)

5.4.3 Summary of Comparisons for TEST 1 and TEST 2

Table 5-6 presents a summary of the comparisons between SUTRA-Bubble predictions and the experimental results from TEST 1 and TEST 2. The good agreement between the predicted and experimental results is a validation of SUTRA-Bubble.
Table 5-6 Validation of SUTRA-Bubble with Glass Tank IPS Experimental Tests

<table>
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<th>Sets of Results</th>
<th>Experiment TEST 1 1% Conc.</th>
<th>SUTRA-Bubble TEST 1 1% Conc.</th>
<th>Experiment TEST 2 0.5% Conc.</th>
<th>SUTRA-Bubble TEST 2 0.5% Conc.</th>
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</thead>
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</tr>
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<td>Long After Injection</td>
<td>19898</td>
<td>21947</td>
<td>13700</td>
<td>15640</td>
</tr>
<tr>
<td><strong>Pore Water Pressures (cm)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PPT1</td>
<td>46</td>
<td>39</td>
<td>45</td>
<td>44</td>
</tr>
<tr>
<td>PPT2</td>
<td>45</td>
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<td>44</td>
<td>44</td>
</tr>
<tr>
<td>PPT3</td>
<td>40</td>
<td>35</td>
<td>41</td>
<td>36</td>
</tr>
<tr>
<td>PPT4</td>
<td>30</td>
<td>27</td>
<td>30</td>
<td>27</td>
</tr>
<tr>
<td>PPT5</td>
<td>24</td>
<td>22</td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td><strong>Zone of Influence (cm)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Concentration</td>
<td>25</td>
<td>24-27</td>
<td>20</td>
<td>22-24</td>
</tr>
<tr>
<td>Degree of Saturation</td>
<td>30</td>
<td>27-31</td>
<td>25</td>
<td>25-28</td>
</tr>
<tr>
<td><strong>Degree of Saturation (%)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Range</td>
<td>59-73</td>
<td>55-58</td>
<td>54-77</td>
<td>75-78</td>
</tr>
<tr>
<td>Average</td>
<td>65</td>
<td>57</td>
<td>69</td>
<td>76</td>
</tr>
</tbody>
</table>
Chapter 6

Comparison of SUTRA-Bubble Predictions with Results of Large Scale Induced Partial Saturation Experiment: Laminar Box

6.1 Overview

Chapter 5 presented details of Induced Partial Saturation (IPS) experiments performed on sand specimens prepared in a large glass tank. In addition, details of SUTRA-Bubble simulations were presented and results similar to those measured in the experiments were predicted. Comparisons were made between the predicted and measured results for the purpose of validating SUTRA-Bubble.

A further validation of SUTRA-Bubble was made by using results from a large scale IPS experiment performed on a sand specimen that was prepared in the Laminar Box of SUNY at Buffalo (NEES@Buffalo site). In this chapter, a brief explanation of the IPS project that was conducted using the Laminar Box is presented, followed by relevant experimental test results obtained for use in the validation of SUTRA-Bubble. The chapter also presents SUTRA-Bubble simulations of IPS tests performed in the Laminar Box and concludes with the comparisons of predicted and measured results.
6.2 Induced Partial Saturation Experiment in Laminar Box

The laminar Box at the NEES@Buffalo site is a large (2-story) steel box, which allows testing of sands under real free-field seismic ground motions. This NEESR IPS project included seismic testing of partially saturated sands using the Laminar Box. Such testing required the preparation of partially saturated sand specimens in the box and then shaking the specimens to determine the effect of partial saturation on the liquefaction resistance of sands. The preparation of a partially saturated sand in the laminar box entailed injection of sodium percarbonate solution, and through flow and reactivity generate gas bubbles, thus reducing the degree of saturation of the initially fully saturated sand specimen, in a manner similar to the glass tank experiments described in Chapter 5. SUTRA-Bubble was used to design an optimal process of IPS including determination of spacing of the injection tubes, injection pressure, and injection duration. The validity of the SUTRA-Bubble predictions of zone of partial saturation and degree of saturation were later evaluated by using electric conductivity probe measurement data obtained during and long after injection of the solution.

6.2.1 Laminar Box Experiment

The Laminar Box is composed of 39 laminates (I-beam-cross sections) stacked vertically to form a rectangular box. It can be assembled to a maximum height of 6 meters, which allows the preparation of a soil specimen of 5 meters in height. The nominal internal dimensions of the box are 5 meters in length and 2.75 meters in width. In the test described herein, the dimensions of the sand specimen prepared were 5 m x 2.75 m x 5 m. Figure 6-1 shows pictures of the Laminar Box and top of the sand specimen in the box. The box was instrumented with pore pressure transducers, accelerometers, displacement
transducers for measurements during shaking to analyze soil liquefaction, as well as with electrical conductivity probes to estimate the degree of saturation at all times starting injection, gas generation, and after shaking.

Figure 6-1(a) 2-story tall Laminar Box IPS set-up (b) top of a sand specimen

The system for preparation and injection of sodium percarbonate solution can be seen in Figure 6-1 (a) and Figure 6-2 (a). The system includes a water source connected to one or more barrels, where the sodium percarbonate solution is mixed to a certain concentration, and a constant pressure pump sends the solution to an injection tube inserted in the sand specimen. Figure 6-2 (b) shows the injection tube, which is perforated near its tip. A perforated closed-ended tube was preferred over an open-ended tube without perforations in order to create lateral flow of solution to achieve larger zone of partial saturation. It is noted that the perforation near the tip was also modelled in the SUTRA-Bubble simulation of inducing partial saturation in the Laminar Box sand specimen.
The volume of sand to be treated with IPS was large (approximately 68.75 m$^3$), which required employment of 31 injection locations both vertically and horizontally. Figure 6-3 shows the injection locations in plan view. Figure 6-3 (b) shows that the box was treated in two stages in elevation. Due to the limitation of the head room at the top of the box and the length of the injection tube; first the bottom 10 feet of the box was treated with the chemical solution. Then, the top 6 feet was treated with a similar but shorter injection tube. The bottom injection was completed from locations 1 to 13. The top injection was completed from locations 14 to 31. The bottom injection was performed by jetting the injection tube down to 1 foot above the bottom of the sand specimen, and solution was pumped for a certain period of time, until nearby electric conductivity probes registered the arrivals of the solution. Then, without stopping pumping of the solution, the injection tube was lifted by 1-ft and held there again for a certain period of time. This procedure was continued until the entire bottom of the sand specimen was treated. The same procedure was followed to treat the top portion of the specimen.
Figure 6-3 Locations of 31 injections performed for treating the bottom and top of the sand specimen in the Laminar Box

SUTRA-Bubble simulation of the treatment of the entire sand specimen was deemed not practical and unnecessary. For the purpose of validation of SUTRA-Bubble,
the experimental results measured during only the first injection location, with the multiple lifts, were used.

### 6.2.2 Degree of Saturation Results from Laminar Box Experiment

Similar to the glass tank experiments presented in Chapter 5, changes in degree of saturation in the sand specimen during and after injection of sodium percarbonate solution were detected by the electrical conductivity probes placed in the Laminar Box (Figure 6-4). A total of 21 electrical conductivity probes were used most of them next to the pore pressure transducers, in order to determine the degree of saturation around the pressure transducers. Pore pressure measurements during shaking of the specimen in the Laminar Box were needed to determine the effectiveness of IPS as a liquefaction mitigation measure.

![Electrical Conductivity probe with a long cables, inserted in the laminar box specimen](image)

Figure 6-4 Typical electrical conductivity probe with a long cables, inserted in the laminar box specimen

The locations of these 21 electrical conductivity probes in both plan and elevation are presented in Figure 6-5. The probes that were inside the area planned for SUTRA-Bubble simulation are highlighted with arrows in Figure 6-5.
The calculation procedure for degree of saturation based on electric conductivity measurements was described in Chapter 5. Figure 6-6 presents electric conductivity readings of the probes in the vicinity of injection location 1. The degree of saturation at each probe location, 2 to 3 hours after injection is indicated on each probe plot.
Figure 6-6 Degree of saturation at each probe location within the planned simulation area

Figure 6-6 shows that the estimated degree of saturation at probes CP1 and CP2, which was very close to Injection 1 were 67% and 64%, respectively. During Injection 1, the solution arrived also at probes CP4 and CP5, which were approximately 0.8 meters away from Injection 1, and the degree of saturation were about 81% and 92%, respectively.
Finally, it appears that the solution did not arrive at probes CP12 and CP13, which were approximately 1.2 meters away from Injection 1, which indicates that the sand around these probes remained fully saturated. Therefore, assuming a circular zone of treatment, a partial saturation zone with a radius between 0.8 and 1.2 meters from Injection 1 is presumed (Figure 6-7).

Figure 6-7 Zone of partial saturation around Injection 1 in plan view of the box
6.3 SUTRA-Bubble Simulation of Laminar Box Sand Specimen

As mentioned in the previous section, only the first injection (Injection 1) in the Laminar Box was simulated with SUTRA-Bubble. Figure 6-8 shows the simulated area in the plan view of the box, which is around Injection 1 and is limited to 3m x 2.75m in plan and 5 m (the height of the soil) in elevation. The simulated area was considered large enough to properly observe the flow created by Injection 1.

Figure 6-8 Portion of the sand specimen simulated in SUTRA-Bubble

The three-dimensional (3D) mesh that was created for the Laminar Box simulation is shown in Figure 6-9. The injection nodes representing the perforated tip of the injection tube are highlighted in the figure. Five lifts of the injection tube were simulated, covering the portion of the sand where the probes that provided degree of saturation data were located (CP1-2, CP4-5, and CP12-13). At each lift, the constant injection pressure that was measured during the injection was assigned at the injection nodes. Similar to other SUTRA-Bubble simulations, the top of the soil was assigned with a zero water pressure boundary condition representing free water surface. This is consistent with the fact that
during injection of the solution, the water on top of the sand in the Laminar Box was pumped out.

**3D view of the SUTRA-Bubble mesh**

The simulation parameters included: injection pressure, design concentration, duration of injection at each lift, porosity, dispersivity, and permeability of the sand. It is known that the most important parameter for SUTRA-Bubble simulation is soil permeability, which has a direct effect on flow and transport of solution. The following section discusses the determination of the saturated permeability of the sand specimen prepared in the Laminar Box.
6.3.1 Determination of Saturated Permeability of Sand Specimen in Laminar Box

The sand used in the Laminar Box was Ottawa F55 purchased from U.S. Silica Company. NEES@Buffalo measured the saturated permeability of the Ottawa F55 sand using laboratory apparatus for 1D permeability test. Table 6-1 presents the test results of permeability tests at two different void ratios using F55 Ottawa sand.

Table 6-1 Laboratory data for permeability for F55 Ottawa sand

<table>
<thead>
<tr>
<th>1-D Permeability Test</th>
<th>Void Ratio</th>
<th>Permeability, cm/s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.67</td>
<td>0.026</td>
</tr>
<tr>
<td></td>
<td>0.69</td>
<td>0.035</td>
</tr>
</tbody>
</table>

In addition, a flow rate test was conducted by the Northeastern University team in the Laminar Box to determine in-situ saturated permeability of the sand specimen. The flow rate test was conducted on a fully saturated sand specimen that was prepared for a preliminary IPS test using the Laminar Box. The experimental test set-up that was used in the flow rate test is presented in Figure 6-10. The injection set-up utilized six 1 inch diameter open ended injection tubes hung in the box, before the placement of the sand, with their tips about 3 meters from the top of the sand specimen, and covered with geotextile. The previously described injection system was used to pump clean water under constant pressure. During the injection of clean water, a constant pressure was applied and the flow rates of the clean water were measured. The measured data of flow rates are presented in Table 6-2.
Using the measured data of applied injection pressure and flow rate, SUTRA-Bubble simulation was performed to back-figure the saturated permeability of the sand specimen prepared in the Laminar Box.

![Injection system](Image)
![Injection tubes inserted in sand](Image)

**Figure 6-10** Experimental set-up for water injection test in the Laminar Box

<table>
<thead>
<tr>
<th>Flow rate test measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Applied injection pressure at every 6 injection tubes</td>
</tr>
<tr>
<td>Measured flow rate for total 6 injection tubes</td>
</tr>
<tr>
<td>10.5 psi</td>
</tr>
<tr>
<td>22.3 gpm</td>
</tr>
</tbody>
</table>

**Table 6-2 Measured data for flow rate test in Laminar Box**

The SUTRA-Bubble mesh that was prepared for the flow rate test conducted in the Laminar Box is presented in Figure 6-11. The 6 injection tubes that were 3 m deep in the sand specimen were modeled with square elements. Very low permeability values were assigned at those elements to simulate the injection tubes. The area of each element was 5 cm² equivalent to the open area at the tip of an injection tube. The measured input pressure was assigned as specified pressure boundary condition at the injection nodes. SUTRA-Bubble outputs for the total flow rate were matched with the measured values by changing the value of the saturated permeability. This calibrated value was determined to be 0.048
cm/s for a void ratio of 0.73. The void ratio was measured by NEES@Buffalo during the placement of the sand in the Laminar Box.

\[
\text{Input pressure} = 10.5 \text{ psi}
\]
\[
\text{Matched output of flow rate} = 22.3 \text{ gpm (6 holes)}
\]
\[
\text{with } k = 0.048 \text{ cm/s}
\]
\[
e = 0.73 \text{ for } D_r = \sim 40\%
\]

Figure 6-11 SUTRA-Bubble mesh for flow rate test in the Laminar Box

The permeability value calibrated from SUTRA-Bubble simulation and the two laboratory data from 1D experiment were compared. However, the measured void ratios for the permeability values were different; the voids ratios of the two laboratory data were 0.67 and 0.69, and the void ratio of the sand in the Laminar Box was 0.73. Therefore, Kozeny-Carman equation was used to plot permeability versus void ratio based on the two measured data from 1D permeability experiment. The back-figured value for the sand in the Laminar Box was then plotted with these two curves for comparison. Equation (6-1) shows the Kozeny-Carman equation which relates permeability to void ratio. Figure 6-12 show the two separate curves, anchored at the two 1D data, and the back-figured value from SUTRA-Bubble.
\[
\frac{k_1}{k_2} = \frac{e_1^3}{(1+e_1)} \frac{e_2^3}{(1+e_2)}
\]  
(Kozeny-Carman Equation)  

(6-1)

where:

\(k_1\) = permeability for the measured data

\(e_1\) = void ratio for the measured data

\(k_2\) = subsequent permeability to be calculated

\(e_2\) = subsequent void ratio to be used in calculation

The back-calculated permeability value from SUTRA-Bubble simulation was slightly larger than the predicted values of the extrapolated portions of the two curves, at void ratio of 0.73. It is noted that the back-figured value was based on in-situ measurements specific to the sand specimen prepared in the Laminar Box whereas the curves were based on 1D data obtained from a different experimental set-up. Therefore the back-figured value of 0.048 cm/s was used in the SUTRA-Bubble simulation.

![Figure 6-12 Permeability of sand specimen in the Laminar Box](image-url)
6.3.2 Modeling of Perforated Injection Tube

A perforated injection tube was used to achieve lateral flow and transport of solution leading to laterally larger zone of partial saturation. Perforation was made by drilling holes uniformly distributed within the bottom 1 foot of the injection tube, resulting in a total opening of 10% of the surface area of the 1 foot length of the tube. The most appropriate approach to simulate the perforation at the tip of the tube was to assign multiple layers with specified pressure nodes and certain z discretization for a total length of 1 foot. Considering the number of 1 foot lifts performed during injection, a reasonable number of lifts as well as reasonable number of layers per 1 foot opening was decided. For this purpose, only five of the 1 foot lifts (from a total of 9 lifts) were simulated. The simulation of 5 lifts was deemed adequate to capture the transport and the reduction in saturation in the region of the conductivity probes that provided the experimental data. Each 1 foot lift was divided into 5 layers to simulate the perforated opening on the injection tube. At each of these 5 layers, constant pressure for injection was assigned at injection nodes. Figure 6-13 shows the sketch of the injection nodes at 5 layers representing the 1 foot perforated opening of the injection tube. The injection nodes were assigned at the four corners of the square no-flow block that was created to represent the injection tube. Since there was no flow into the square block the injection nodes allowed flow from the sides of the block representing the lateral flow. The open surface area around the perimeter of each square block was the cross sectional area of the flow. This simulated open area is described on the sketch by the red shaded zone (Figure 6-13). However, it is critical to note that the height required to calculate the surface area around the perimeter of the square block depends on whether the layer is divided into finer elements using Z discretization or not.
Therefore, the reasonable numbers for the two dimensions; 1) size (perimeter) of the square block and 2) z discretization were determined by equating the total open area on the surface of the injection tube to the total open surface area in the simulation.

Figure 6-13 Modeling of perforated injection tube

The open area on the injection tube was estimated to be 10% of the total surface area for 1 foot length. The calculations to determine the size of the square block, representing the size of the injection tube, and z discretization representing the size of the opening in z direction are presented below.

open area on the tube = 0.10 x total surface area of 1 foot of the tube = 24 cm²

24 cm² = (perimeter of the square block x thickness in z) x 5

Thickness in Z direction = 1.524 cm

Perimeter of the square opening = 3.1 cm
Very small values for the thickness in Z was computationally very time consuming, and a very small opening for the injection tube would not be representative of the size of the injection tube. The values presented above were calculated for the thickness in Z direction and the size of the square block representing the injection tube and were found to be reasonable taking all the limitations into account. It is noted that the simulated open area was continuous around the perimeter of the square block, whereas the real perforation on the injection tube was composed of discrete holes drilled on the surface of the tube. The square block representing the injection tube with a perimeter of 3.1 cm is shown on the plan view of the SUTRA-Bubble mesh in Figure 6-14.

Figure 6-14 Plan view of SUTRA-Bubble mesh showing the injection tip opening

In summary, the SUTRA-Bubble mesh that was created to simulate first injection location (Injection 1) of the IPS experiment in the Laminar Box together with the essential parameters for injection are shown in Figure 6-15. The injection pressure for each lift of the injection tube was 20 psi and the duration of injection ranged between 2 and 4 minutes for each lift. The design concentration of the chemical solution was 1% by weight. A list of the input parameters used in SUTRA-Bubble simulation of the IPS experiment in the Laminar Box is shown in Table 6-3.
Input pressure at each lift = 20 psi

Input permeability - $k = 0.048 \text{ cm/s}$

3-D view of the SUTRA-Bubble mesh

Elevation view of the SUTRA-Bubble mesh

Figure 6-15 SUTRA-Bubble mesh of IPS experiment in the Laminar Box (a) 3D (b) elevation
Table 6-3 List of input parameters used in SUTRA-Bubble simulation of IPS experiment in the Laminar Box

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size of model</td>
<td>3 m (L) x 2.75 cm (W)</td>
</tr>
<tr>
<td>Specimen height</td>
<td>5 m</td>
</tr>
<tr>
<td>Depth of Injection tip</td>
<td>Starts at 4.574 m increases with each lift</td>
</tr>
<tr>
<td>Porosity</td>
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</tr>
<tr>
<td>Average Saturated Permeability</td>
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</tr>
<tr>
<td>Dispersivity (Long. &amp; Trans.)</td>
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</tr>
<tr>
<td>Diffusion coefficient</td>
<td>1E-9 m²/s</td>
</tr>
<tr>
<td>Coefficient of density change ( \frac{\hat{c}_p}{\hat{c}_C} )</td>
<td>4052 (kg/m³)</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>Hydrostatic pressure</td>
</tr>
<tr>
<td>Initial concentration</td>
<td>0 (kg/kg)</td>
</tr>
<tr>
<td>Injection pressure</td>
<td>20 psi</td>
</tr>
<tr>
<td>Actual concentration of H₂O₂ solution (C₃H₂O₅) actual</td>
<td>0.002468 (kg/kg)</td>
</tr>
<tr>
<td>Duration of injection</td>
<td>Average 2 to 4 min at each lift</td>
</tr>
<tr>
<td></td>
<td>Total 18 minutes for 5 lifts</td>
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<tr>
<td>Total duration of the model</td>
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</tr>
<tr>
<td>Time increment</td>
<td>1 minute (for 30 minutes)</td>
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<tr>
<td></td>
<td>5 minutes (30 to 180 minutes)</td>
</tr>
<tr>
<td></td>
<td>25 minutes (180 to 330 minutes)</td>
</tr>
<tr>
<td>Mesh size in plan</td>
<td>3 cm around injection (1.5 m x 1.5 m square zone)</td>
</tr>
<tr>
<td></td>
<td>6 cm away from injection</td>
</tr>
<tr>
<td>Z discretization</td>
<td>1.524 cm to 18 cm</td>
</tr>
<tr>
<td></td>
<td>Fine discretization is needed for perforation</td>
</tr>
<tr>
<td>Number of nodes</td>
<td>744464</td>
</tr>
<tr>
<td>Number of elements</td>
<td>725625</td>
</tr>
<tr>
<td>Solver for pressure</td>
<td>Iterative – CG</td>
</tr>
<tr>
<td></td>
<td>Tolerance – 1E-13</td>
</tr>
<tr>
<td></td>
<td># of iterations - 1000</td>
</tr>
<tr>
<td>Solver for pressure</td>
<td>Iterative – GMRES</td>
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<tr>
<td></td>
<td>Tolerance – 1E-13</td>
</tr>
<tr>
<td></td>
<td># of iterations - 500</td>
</tr>
</tbody>
</table>
6.3.3 SUTRA-Bubble Predictions of IPS Experiment in Laminar Box

In this section, predictions of SUTRA-Bubble simulation are presented using different sectional views from the simulated zone. Three sections were used to present SUTRA-Bubble predictions as shown in Figure 6-16. The sections are at the probe locations in order to observe the transport of the solution as well as the degree of saturation predictions at each probe location.

Figure 6-16 The three sections used to present SUTRA-Bubble predictions (a) Section A-A and B-B in elevation and (b)Section C-C in plan
Section A-A is in elevation at the injection tube and locations of probes CP1, CP2, CP12, and CP13. Section B-B is also in elevation at the locations of probes CP4 and CP5. Section C-C is in plan at the elevation of probe CP4. Concentration outputs of SUTRA-Bubble along Section A-A during the injection process for the total of the five 1-foot lifts of the injection tube are shown in Figure 6-17. The outputs show that the concentration plum moved up with the lifts of the injection tube showing the reasonable simulation of perforated tube at multiple elevations. The total duration of the simulated injection (five lifts) was 18 minutes. At the end of the injection, the bulb of the design concentration (1%) of the injected solution was approximately 1 m wide around the injection tube. The entire concentration bulb around the injection nodes was approximately 1.5 m wide.

Figure 6-17 Concentration output of SUTRA-Bubble for Section A-A during injection process (5 lifts - each 1ft)

The degree of saturation predictions of SUTRA-Bubble along Section A-A after 5 hours (at the end of gas generation) are presented in Figure 6-18. The predictions show that the zone of partial saturation created around the injection nodes was 1.8 meter wide in
the lateral direction. The final degree of saturation created by the design concentration of 1% was around 0.6 (60%).

Figure 6-18 Degree of saturation output of SUTRA-Bubble for Section A-A

Figure 6-19 shows the predicted zone of partial saturation along Section C-C which is a plan view. A symmetric circular zone of partial saturation was predicted from the simulation because the soil and the injection conditions were all ideal, symmetric, and free of boundary effects. The radius of the circular zone of partial saturation was predicted to be around 0.95 meters.
In this section, SUTRA-Bubble predictions are compared with the results obtained by the electrical conductivity measurements within the simulated zone. The degree of saturation values obtained from the electrical conductivity measurements are plotted on the SUTRA-Bubble degree of saturation plots in Figure 6-20 (a) and (b). Along Section A-A, in the region of probes CP-1 and CP-2, the SUTRA-Bubble predicted degree of saturation is about 0.6 (60%), which compares well with the results from Probe CP1, 0.67 (67%) and CP2, 0.64 (64%). The predictions also showed fully saturated conditions at the locations of probes CP12 and CP13, which is consistent with the probe measurements showing that the solution did not reach these probe locations. Along Section B-B, which is 0.5 m from the injection tube, SUTRA-Bubble prediction of degree of saturation at the location of CP-4 was 0.90 (90%), compared with 0.81 (81%) obtained from the probe. The predicted degree of saturation for the location of CP5 was 1.0 (100%) indicating full saturation,
whereas the CP5 indicated a slight partial saturation with a degree of saturation of 0.92 (92%).

Table 6-4 presents a summary of degree of saturation predicted by SUTRA-Bubble and computed based on the conductivity probe measurements. The predicted values are generally in good agreement with the conductivity probe results. The agreement is not as good when the comparison is made at points further away from the injection tube, where the degree of saturation is only slightly less than 1. In such cases, the degree of saturation in both predicted and probe based can be very sensitive to the various assumptions made and parameters used in the simulation.
Comparison of SUTRA-Bubble predictions with probe measurements

Section A-A

Section B-B

Figure 6-20 Comparison of SUTRA-Bubble predictions for degree of saturation with conductivity probe measurements (a) Section A-A (b) Section B-B
Table 6-4 Predicted and measured degree of saturation values at each probe location

<table>
<thead>
<tr>
<th></th>
<th>Conductivity Probe</th>
<th>SUTRA-Bubble</th>
</tr>
</thead>
<tbody>
<tr>
<td>CP 1</td>
<td>0.67</td>
<td>~ 0.60</td>
</tr>
<tr>
<td>CP 2</td>
<td>0.64</td>
<td>~ 0.60</td>
</tr>
<tr>
<td>CP 4</td>
<td>0.81</td>
<td>~ 0.90</td>
</tr>
<tr>
<td>CP 5</td>
<td>0.92</td>
<td>1.00</td>
</tr>
<tr>
<td>CP 12</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>CP 13</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Finally, in Figure 6-21 the radius of the zone of partial saturation predicted by SUTRA-Bubble was compared with the zone estimated by the conductivity probe measurements (Figure 6-7). The probe measurements indicated that the solution arrived and created partial saturation at CP4 and CP5, which were 0.8 meters away from the injection tip, whereas it did not arrive at probes CP12 and CP13, indicating fully saturated conditions. Therefore, the radius of the presumed zone of partial saturation estimated by the probes ranged between 0.8 and 1.2 meters, which compare well with the SUTRA-Bubble predicted zone of partial saturation with a radius of 0.95 meters.
Table 6-5 presents a summary comparison of the SUTRA-Bubble predicted and Laminar Box test results. The degree of saturation and the size of the zone of partial saturation predicted by SUTRA-Bubble agree reasonably well with those determined using electric conductivity measurements. This agreement, using the results from the IPS application in the Laminar Box, is a further validation of the capability of SUTRA-Bubble to make reasonable predictions of 3D transport and reactivity, as well as to provide reasonable estimates of degree of saturation by IPS in sands.

Table 6-5 Validation of SUTRA-Bubble with the Laminar Box IPS Experimental Test

<table>
<thead>
<tr>
<th>Sets of Results</th>
<th>Laminar Box 1% Conc.</th>
<th>SUTRA-Bubble 1% Conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone of Influence (m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Section A-A (largest bulb)</td>
<td>&lt; 2.4</td>
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<td>1.6 - 2</td>
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</tr>
<tr>
<td>Section C-C (radius)</td>
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<td>0.95</td>
</tr>
<tr>
<td>Degree of Saturation (%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CP1</td>
<td>67</td>
<td>~ 60</td>
</tr>
<tr>
<td>CP2</td>
<td>64</td>
<td>~ 60</td>
</tr>
<tr>
<td>CP4</td>
<td>81</td>
<td>~ 90</td>
</tr>
<tr>
<td>CP5</td>
<td>92</td>
<td>100</td>
</tr>
<tr>
<td>CP12</td>
<td>100</td>
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<tr>
<td>CP13</td>
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</table>
Chapter 7

Summary and Conclusions

This dissertation presents the theoretical basis, numerical simulation and experimental verification of Induced Partial Saturation (IPS), an innovative, practical and cost effective new liquefaction mitigation technique developed at Northeastern University (Yegian et al., 2007). Specifically, the research discussed in this dissertation focuses on developing the basic mathematical equations as well as a numerical simulation code for transient gas generation induced through transport and reactivity of sodium percarbonate solution to reduce the degree of saturation in sands that are initially fully saturated. This work is critical for advancing the IPS technology; it will allow engineering of field implementations and determination of the critical design and analysis parameters.

To achieve this goal, the SUTRA-Bubble program - a modified version of the SUTRA program released by Voss, (1984) – is developed. SUTRA simulates two interdependent processes; fluid density dependent saturated or unsaturated flow and transport of a solute in porous media subject to zero and/or first order decay or production. SUTRA is used as the basis for SUTRA-Bubble because it is capable of modeling transport of sodium percarbonate solution, which has a density higher than water, into saturated sand and for computing the associated changes in the degree of saturation. However, the partial saturation conditions induced by IPS are different from those calculated by SUTRA for typical unsaturated conditions in the capillary zone above the water table. In IPS, the gas bubbles generated by the chemical reaction are trapped in the pores of the saturated sand, which is below the water table, are disconnected from the atmosphere, and under positive
pore pressure. Therefore, different physical conditions apply for this type of partial saturation. The SUTRA program was modified employing new theoretical formulations to define the new partial saturation induced by injection of a chemical solution. The following tasks were completed to develop SUTRA-Bubble by modifying SUTRA:

- New formulations were developed, based on the ideal gas law, to calculate changes in the degree of saturation as a function of molar concentration of gas bubbles.
- The required modifications caused by changes in the degree of saturation were implemented on the governing flow equation in SUTRA.
- A constitutive model for the kinetics of gas generation in sand over time was created. The change in molar concentration of gas bubbles, representing the volume of gas generated with time is expressed as a function of the change in solute concentration. The molar concentration of gas bubbles was then solved numerically in the constitutive model using the proper rate parameter for the gas generation reaction. In the SUTRA-Bubble simulations, the solute was hydrogen peroxide, and its concentration determined the rate of gas bubble generation.
- A constitutive model for the reduction in soil permeability due to the presence of bubbles was implemented. The factor by which soil permeability is reduced relative to the fully saturated permeability (the relative permeability) was defined as a power function of the degree of saturation of the soil. The power-law exponent was determined in laboratory experiments.
• The effect of the variable density of the sodium percarbonate solution on the flow was modeled using the original fluid density model in the SUTRA program. This model relates fluid density to the concentration of solute calculated by the program, which is the concentration of hydrogen peroxide in the SUTRA-Bubble simulations. The effect of ions (sodium and carbonate) in the sodium percarbonate solution was disregarded in SUTRA-Bubble, which led to underestimation of the effect of the actual fluid density. This effect was demonstrated to be inconsequential.

In the second phase of the research, the constitutive parameters for the rate of gas generation, reaction efficiency, and relative permeability in sand were determined through small-scale laboratory experiments using Ottawa sand and sodium percarbonate as the gas source. Existing correlations between the relative permeability and degree of saturation were not applicable for the partial saturation conditions created by IPS. The correlations reported in literature (e.g., Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980; Bicalho and Znidarcic, 2000) were all for predicting the degree of saturation in a capillary zone above the water table, whereas in this research a degree of saturation as low as 50% was created below water table under positive pore pressures.

In the third phase of the research, an experimental test set-up was designed and manufactured for injection of sodium percarbonate solution into sand specimens prepared in a large glass tank. Under a controlled pressure and a specific solution concentration, the inflow and outflow rates, pore water pressures, and electric conductivity were measured to determine the zone of partial saturation and the spatially varying degree of saturation. The measurements were summarized as three general sets of results:
o Flow and pressure during injection

o Transport of solution

o Degree of saturation

Two similar tests were conducted with the glass tank experimental set-up. SUTRA-Bubble simulations for these two tests were performed to compare the predicted outputs with the experimental results, for validating the principles of the SUTRA-Bubble code.

Finally, SUTRA-Bubble simulation was performed for a large-scale implementation of IPS in the Laminar Box located at the NEES@Buffalo site, and the simulation predictions were compared with experimental measurements.

The research conducted in this dissertation led to the following conclusions:

- SUTRA-Bubble was successfully formulated by modifying the original governing equations employed in the SUTRA program. The compiled program runs effectively for 3D simulations of IPS. The rate of sodium percarbonate reaction in water was determined to follow exponential decay. The first-order rate parameter available in the SUTRA program was used to relate the gas generation to decay of sodium percarbonate in water. The rate parameter for decay representing the rate of the gas generation reaction was determined to be different for different design concentrations. For each implementation of injection, the corresponding rate parameter needs to be determined experimentally.

- The correlation between relative permeability and degree of saturation was adopted from suggested relationship by Brooks and Corey, 1964. The saturation exponent for partially saturated conditions generated by IPS was determined experimentally.
• Validation of SUTRA-Bubble using the glass tank laboratory experiments showed:
  o Predicted pressures were consistently slightly smaller than the measured pressures because the assumption of uniform soil does not necessarily represent the real laboratory specimen.
  o The predicted sizes for the zone of partial saturation were consistent with the estimated sizes from the experimental measurements. The size of the partial saturation zone was sensitive to the rate of inflow of the injection or the injection pressure.
  o The effect of the fluid density on flow was estimated for 1D vertical flow conditions with conservative assumptions. The fluid density model in SUTRA-Bubble underestimated the extent of the zone of partial saturation in the vertical direction from 4 to 11 cm. Compared to the measured size of the zone of partial saturation, which is approximately 25 to 30 cm in glass tank experiments (Table 7-1) and 80 to 120 cm in Laminar Box experiments (Table 7-2), the under-predicting the zone of partial saturation by a few centimeters due to underestimation of the density effect is inconsequential and will be conservative from practical point of view of IPS implementation.
  o The predicted degree of saturation values were slightly different (approximately 5-10%) than the experimentally measured values.

Table 7-1 summarizes the comparisons made between selected results from the glass tank experiments with the corresponding results predicted by SUTRA-Bubble.
Overall, the agreement is remarkably good, confirming that SUTRA-Bubble was able to properly simulate IPS application in the glass tank sand specimens.

Table 7-1 Validation of SUTRA-Bubble with Glass Tank IPS Experimental Tests

<table>
<thead>
<tr>
<th>Sets of Results</th>
<th>Experiment TEST 1</th>
<th>SUTRA-Bubble TEST 1</th>
<th>Experiment TEST 2</th>
<th>SUTRA-Bubble TEST 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1% Conc.</td>
<td>1% Conc.</td>
<td>0.5% Conc.</td>
<td>0.5% Conc.</td>
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<tr>
<td><strong>Outflow ( gr.)</strong></td>
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<td></td>
<td></td>
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<tr>
<td>End of Injection</td>
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<td>15606</td>
<td>12358</td>
<td>12231</td>
</tr>
<tr>
<td>Long After Injection</td>
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<td><strong>Pore Water Pressures (cm)</strong></td>
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<tr>
<td>PPT1</td>
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<td>39</td>
<td>45</td>
<td>44</td>
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<tr>
<td>PPT2</td>
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<td>PPT3</td>
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<td>41</td>
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<tr>
<td>PPT5</td>
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<td>22</td>
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<tr>
<td><strong>Zone of Influence (cm)</strong></td>
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<td></td>
<td></td>
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<tr>
<td>Concentration</td>
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<td>24-27</td>
<td>20</td>
<td>22-24</td>
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<td>Degree of Saturation</td>
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<td>27-31</td>
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<td>25-28</td>
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<tr>
<td><strong>Degree of Saturation (%)</strong></td>
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<td></td>
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<td>75-78</td>
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<tr>
<td>Average</td>
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<td>57</td>
<td>69</td>
<td>76</td>
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</tbody>
</table>

Predictions of SUTRA-Bubble simulation of IPS in the Laminar Box were also in good agreement with the selected experimental test results, as summarized in Table 7-2.
Table 7-2 Validation of SUTRA-Bubble with the Laminar Box IPS Experimental Test

<table>
<thead>
<tr>
<th>Sets of Results</th>
<th>Laminar Box 1% Conc.</th>
<th>SUTRA-Bubble 1% Conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone of Influence (m)</td>
<td></td>
<td></td>
</tr>
<tr>
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</tr>
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<td>100</td>
</tr>
</tbody>
</table>

This research has demonstrated that the developed computer program SUTRA-Bubble, which is a modified version of SUTRA, is capable to simulate Induced Partial Saturation (IPS) in sands.
REFERENCES


http://water.usgs.gov/nrp/gwsoftware/sutra.html


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