SENSITIVITY AND UNCERTAINTY ANALYSES OF CONTAMINANT FATE AND TRANSPORT IN A FIELD-SCALE SUBSURFACE SYSTEM

A Thesis
Presented to
The Academic Faculty

By

Jinjun Wang

In Partial Fulfillment
Of the Requirements for the Degree
Doctor of Philosophy in Environmental Engineering
School of Civil and Environmental Engineering

Georgia Institute of Technology
April 2008
SENSITIVITY AND UNCERTAINTY ANALYSES OF CONTAMINANT FATE AND TRANSPORT IN A FIELD-SCALE SUBSURFACE SYSTEM

Approved by:

Dr. Mustafa M. Aral, Advisor  
School of Civil and Environmental Engineering  
*Georgia Institute of Technology*

Dr. Jian Luo  
School of Civil and Environmental Engineering  
*Georgia Institute of Technology*

Dr. Seong Hee Kim  
School of Industrial and Systems Engineering  
*Georgia Institute of Technology*

Dr. Jiabao Guan  
School of Civil and Environmental Engineering  
*Georgia Institute of Technology*

Dr. Turgay Uzer  
School of Physics  
*Georgia Institute of Technology*

Date Approved: March 27, 2008
To Emily
ACKNOWLEDGMENTS

In the first place, I would like to express my gratitude to Dr. Mustafa Aral, my advisor at Multimedia Environmental Simulations Laboratory (MESL), for all his support, guidance, and encouragement. During the past years I have learned a lot from Dr. Aral, which is much more than how to conduct research, and which will benefit me through my whole life.

I am deeply indebted to my committee member Dr. Jiabao Guan. His inspiring words have led to many ideas presented in this work. I am also indebted to my committee members Dr. Jian Luo, Dr. Seong Hee Kim, and Dr. Turgay Uzer for their time and effort in reviewing this work.

I am grateful to Morris Maslia and Rene Suarez-Soto from Agency for Toxic Substances and Disease Registry (ATSDR) for their invaluable assistance on the Camp Lejeune project.

My sincere thanks go to all MESL members. Their friendship made my time at MESL very enjoyable. My special thanks go to Scott Rogers, who as my officemate was always there to help.

Last but not least, I would like to thank my parents and my wife, Jie. Without their endless love and unconditional support, this work would have been an impossible mission. My daughter Emily was born right before I finished this thesis. She has brought us lots of laughter and happiness. This thesis is dedicated to her.
TABLE OF CONTENTS

ACKNOWLEDGMENTS ........................................................................................................ iv

LIST OF TABLES .................................................................................................................. viii

LIST OF FIGURES ............................................................................................................... x

LIST OF ABBREVIATIONS ................................................................................................ xv

SUMMARY .......................................................................................................................... xvii

CHAPTER 1: INTRODUCTION ............................................................................................... 1
  1.1 Background .................................................................................................................... 1
  1.2 Motivation and Objective ............................................................................................ 2
  1.3 Organization of the Thesis .......................................................................................... 4

CHAPTER 2: LITERATURE REVIEW ...................................................................................... 6
  2.1 S/O Approach and Its Application to Groundwater Remediation Problems .... 6
  2.1.1 Aquifer Simulation Models .................................................................................... 7
  2.1.2 Formulation of Optimization Problems ................................................................. 9
  2.1.3 Incorporation of Simulation Models ..................................................................... 10
  2.1.4 Optimization Techniques ..................................................................................... 11
  2.2 MODFLOW and MT3DMS ....................................................................................... 13
  2.2.1 MODFLOW .......................................................................................................... 13
  2.2.2 MT3DMS .............................................................................................................. 16
  2.3 Optimization Methods Applied to Groundwater Study ...................................... 18
  2.3.1 Classical Mathematical Programming Methods .................................................. 18
  2.3.1.1 Linear Programming ....................................................................................... 19
  2.3.1.2 Nonlinear Programming ................................................................................ 20
  2.3.1.3 Control Theory Algorithms ......................................................................... 23
  2.3.1.4 Successive Approximation Method ................................................................. 26
  2.3.2 Heuristic Optimization Methods ......................................................................... 27
  2.3.2.1 Genetic Algorithms ......................................................................................... 28
  2.3.2.2 Simulated Annealing ....................................................................................... 30
  2.3.2.3 Tabu Search ..................................................................................................... 32
  2.3.2.4 Derandomized Evolution Strategy ................................................................. 33
  2.3.3 Hybrid Methods .................................................................................................. 34
  2.4 S/O Application under Uncertainty ......................................................................... 37
  2.4.1 Chance-Constrained Approach ......................................................................... 38
  2.4.2 Geostatistical Approach ..................................................................................... 40
  2.4.3 Feedback Control Approach .............................................................................. 42
  2.4.4 Fuzzy Sets Approach .......................................................................................... 43
  2.5 Sensitivity Analysis and Uncertainty Analysis ....................................................... 44
CHAPTER 3: SENSITIVITY ANALYSIS OF CAMP LEJEUNE MODEL 

3.1 Introduction to Camp Lejeune Model ........................................... 57
3.1.1 Historical Background .......................................................... 57
3.1.2 Simulation Results of ATSDR Modeling Study ....................... 61
3.2 Sensitivity Analyses of Uncertain Variables in Camp Lejeune Model .... 65
3.2.1 Uncertain Variables Identification ......................................... 65
3.2.2 Sensitivity Analyses of Uncertain Variables in Camp Lejeune Model .... 66
3.2.2.1 Storage Coefficient ......................................................... 68
3.2.2.2 Hydraulic Conductivities ................................................ 72
3.2.2.3 Recharge Rate ..................................................................... 81
3.2.2.4 First Order Reaction Rate .................................................. 82
3.2.2.5 Mass Loading Rate ............................................................ 85
3.2.2.6 Bulk Density ...................................................................... 87
3.2.2.7 Longitudinal Dispersivity ................................................... 88
3.2.2.8 Effective Porosity ............................................................... 90
3.2.2.9 Summary of Sensitivity Analysis Results ......................... 92
3.3 Summary ..................................................................................... 93

CHAPTER 4: EFFECT OF PUMPING SCHEDULE VARIATION ON CONTAMINANT CONCENTRATIONS AND ARRIVAL TIMES ............ 96
4.1 Optimization Problem .................................................................. 98
4.2 Methodology of PSOpS ............................................................... 100
4.2.1 Rank-and-Assign Method ....................................................... 102
4.2.2 Improved Gradient Method .................................................... 104
4.3 Application of PSOpS to a Simple Case ...................................... 106
4.4 Application of PSOpS to Camp Lejeune Model ............................. 110
4.4.1 Optimization and Simulation Results for the Maximum Schedule .... 110
4.4.1.1 PCE Distribution in the Groundwater System .................. 112
4.4.1.2 PCE Concentration at Water-Supply Wells ..................... 116
4.4.1.3 PCE Concentration at the WTP ...................................... 119
4.4.2 Optimization and Simulation Results for Minimum Schedule I .... 123
4.4.2.1 PCE Distribution in the Groundwater System .................. 124
4.4.2.2 PCE Concentration at Water-Supply Wells ..................... 129
4.4.2.3 PCE Concentration at the WTP ...................................... 131
4.4.3 Optimization and Simulation Results for Minimum Schedule II .... 134
4.4.3.1 PCE Distribution in the Groundwater System .................. 135
4.4.3.2 PCE Concentration at Water-Supply Wells ..................... 143
4.4.3.3 PCE Concentration at the WTP ...................................... 145
4.4.4 Summary of Simulation Results .......................................................... 148
4.4.4.1 Pumping Rate in Well TT-26 ......................................................... 148
4.4.4.2 PCE Concentration at Well TT-26 ................................................. 150
4.4.4.3 PCE Concentration at the WTP ..................................................... 152
4.5 Summary ............................................................................................... 154

CHAPTER 5: UNCERTAINTY ANALYSIS OF CAMP LEJEUNE MODEL .......... 158
5.1 Introduction to Monte Carlo Simulation .................................................. 159
5.1.1 Filtering Process .................................................................................. 161
5.1.2 Statistical Module .............................................................................. 162
5.2 Generation of Input Data ........................................................................ 163
5.2.1 Generation of Hydraulic Conductivities .............................................. 164
5.2.2 Generation of Pumping Schedules ....................................................... 168
5.2.3 Generation of Other Uncertain Variables ........................................... 173
5.3. Simulation Results and Discussion ....................................................... 176
5.3.1 MCS Results of Scenario 1 ................................................................. 176
5.3.2 MCS Results of Scenario 2 ................................................................. 181
5.3.3 Comparison of MCS Results for Scenario 1 and Scenario 2 .............. 185
5.4 Summary ............................................................................................... 190

CHAPTER 6: EVALUATION OF CONTAMINANT ARRIVAL TIMES UNDER
MULTI-PARAMETER UNCERTAINTIES ..................................................... 192
6.1 Introduction ............................................................................................ 192
6.2 Methodology of PDCRI ......................................................................... 195
6.3 Verification of PDCRI ............................................................................ 199
6.3.1 Improvement of Reliability vs. Number of Realizations .................... 202
6.3.2 Improvement of Reliability vs. Number of Scenarios ....................... 206
6.4 Application of PDCRI to Camp Lejeune Model ..................................... 207
6.5 Summary ............................................................................................... 211

CHAPTER 7: CONCLUSIONS .................................................................... 214

APPENDIX A: PROOF OF RAA METHOD RESULTS SATISFYING KUHN-
TUCKER CONDITIONS ............................................................................... 219

REFERENCES ......................................................................................... 222
LIST OF TABLES

Table 3.1. Locations and service periods of water-supply wells in Tarawa Terrace area 61
Table 3.2. Sensitivity analysis results for specific yield in layer 1.......................... 70
Table 3.3. Sensitivity analysis results for storage coefficient in layer 2.................... 71
Table 3.4. Ratios of $K_{H(k,i,j)}$ to $K_{V(k,i,j)}$ in Camp Lejeune model .................. 72
Table 3.5. Sensitivity analysis results for hydraulic conductivities in layer 1............. 74
Table 3.6. Sensitivity analysis results for hydraulic conductivities in layer 2............. 75
Table 3.7. Sensitivity analysis results for hydraulic conductivities in layer 3............. 76
Table 3.8. Sensitivity analysis results for hydraulic conductivities in layer 4............. 77
Table 3.9. Sensitivity analysis results for hydraulic conductivities in layer 5............. 78
Table 3.10. Sensitivity analysis results for hydraulic conductivities in layer 6.......... 79
Table 3.11. Sensitivity analysis results for hydraulic conductivities in layer 7.......... 80
Table 3.12. Sensitivity analysis results for recharge rate.................................... 81
Table 3.13. Sensitivity analysis results for first order reaction rate......................... 83
Table 3.14. Sensitivity analysis results for distribution coefficient.......................... 85
Table 3.15. Sensitivity analysis results for mass loading rate ................................ 86
Table 3.16. Sensitivity analysis results for bulk density...................................... 88
Table 3.17. Sensitivity analysis results for longitudinal dispersivity ....................... 89
Table 3.18. Sensitivity analysis results for effective porosity................................. 91
Table 3.19. Summary of sensitivity analyses results for all uncertain variables ......... 92
Table 4.1. Values of parameters used in the example problem ............................. 107
Table 4.2. PSOpS results summary for the example problem ............................... 109
Table 4.3. PCE concentrations at well TT-26 under the Original Schedule and the
  Maximum Schedule during POI ................................................................. 119
Table 4.4. PCE masses withdrawn under the Original Schedule and the Maximum Schedule ................................................................. 122

Table 4.5. PCE concentrations at the WTP under the Original Schedule and the Maximum Schedule during POI ................................................................. 122

Table 4.6. PCE masses withdrawn under the Original Schedule and Minimum Schedule I ................................................................. 133

Table 4.7. PCE concentrations at the WTP under the Original Schedule and Minimum Schedule I during POI ................................................................. 134

Table 4.8. PCE masses withdrawn under the Original Schedule, Minimum Schedule I, and Minimum Schedule II ................................................................. 147

Table 4.9. PCE concentrations at the WTP under the Original Schedule, Minimum Schedule I and Minimum Schedule II during POI ................................................................. 148

Table 4.10. PCE concentrations and MCL arrival times at well TT-26 under the Original and updated pumping schedules during POI ................................................................. 151

Table 4.11. PCE concentrations and MCL arrival times at the WTP under the Original and updated pumping schedules during POI ................................................................. 153

Table 4.12. PCE masses withdrawn under the Original and updated pumping schedules ................................................................. 153

Table 5.1. Locations of observation points for the filtering process ......................... 162

Table 5.2. Historical pumping demand at Tarawa Terrace ................................................................. 169

Table 5.3. $Q_{T\text{-monthly}}/Q_{T\text{-yearly}}$ ratios at Tarawa Terrace ................................................................. 169

Table 5.4. Statistical results of $Q_{T\text{-monthly}}/Q_{T\text{-yearly}}$ ratios at Tarawa Terrace ................................................................. 170

Table 5.5. Statistical properties of uncertain variables used in uncertainty analysis ...... 176

Table 6.1. Values of parameters used in the example problem ................................................................. 201

Table 6.2. Reliabilities of critical realizations with CI values greater than 0.90 and 0.95 for the example problem ................................................................. 203

Table 6.3. Refreshment Rates of critical realizations for the example problem ................. 206
LIST OF FIGURES

Figure 3.1. Water-supply well locations at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina................................................................. 58

Figure 3.2. Illustration of PCE concentration calculation in Camp Lejeune model........ 62

Figure 3.3. PCE concentrations at water-supply wells under the Original Schedule ...... 63

Figure 3.4. PCE concentrations at the WTP under the Original Schedule ................. 64

Figure 3.5. Uncertain variables applied in Camp Lejeune model............................. 66

Figure 3.6. Sensitivity analysis results for specific yield in layer 1 ......................... 69

Figure 3.7. Sensitivity analysis results for storage coefficient in layer 2 ................. 71

Figure 3.8. Sensitivity analysis results for hydraulic conductivities in layer 1 .......... 74

Figure 3.9. Sensitivity analysis results for hydraulic conductivities in layer 2 .......... 75

Figure 3.10. Sensitivity analysis results for hydraulic conductivities in layer 3 ....... 76

Figure 3.11. Sensitivity analysis results for hydraulic conductivities in layer 4 ....... 77

Figure 3.12. Sensitivity analysis results for hydraulic conductivities in layer 5 ....... 78

Figure 3.13. Sensitivity analysis results for hydraulic conductivities in layer 6 ....... 79

Figure 3.14. Sensitivity analysis results for hydraulic conductivities in layer 7 ....... 80

Figure 3.15. Sensitivity analysis results for recharge rate ........................................ 82

Figure 3.16. Sensitivity analysis results for first order reaction rate .................... 83

Figure 3.17. Sensitivity analysis results for distribution coefficient ...................... 84

Figure 3.18. Sensitivity analysis results for mass loading rate ............................ 86

Figure 3.19. Sensitivity analysis results for bulk density .................................... 87

Figure 3.20. Sensitivity analysis results for longitudinal dispersivity .................. 90

Figure 3.21. Sensitivity analysis results for effective porosity ......................... 91

Figure 4.1. Flowchart of PSOpS ................................................................. 101
Figure 4.2. Flowchart of the Rank-and-Assign method .................................................. 103

Figure 4.3. Flowchart of the Improved Gradient method .................................................. 105

Figure 4.4. Initial contaminant concentration and pumping well distributions for the example problem .......................................................... 107

Figure 4.5. Pumping rate and pumping capacity of well TT-26 under the Maximum Schedule .......................................................... 111

Figure 4.6. Comparison of PCE distribution in Layer 1 under the Original Schedule and the Maximum Schedule .......................................................... 113

Figure 4.7. Comparison of PCE distribution in Layer 3 under the Original Schedule and the Maximum Schedule .......................................................... 114

Figure 4.8. Comparison of PCE distribution in Layer 5 under the Original Schedule and the Maximum Schedule .......................................................... 115

Figure 4.9. PCE concentrations at water-supply wells under the Original Schedule and the Maximum Schedule .......................................................... 117

Figure 4.10. PCE concentrations at the WTP under the Original Schedule and the Maximum Schedule .......................................................... 120

Figure 4.11. Pumping rate and pumping capacity of well TT-26 under Minimum Schedule I .......................................................... 124

Figure 4.12. Comparison of PCE distribution in Layer 1 under the Original Schedule and Minimum Schedule I .......................................................... 126

Figure 4.13. Comparison of PCE distribution in Layer 3 under the Original Schedule and Minimum Schedule I .......................................................... 127

Figure 4.14. Comparison of PCE distribution in Layer 5 under the Original Schedule and Minimum Schedule I .......................................................... 128

Figure 4.15. PCE concentrations at water-supply wells under the Original Schedule and Minimum Schedule I .......................................................... 129

Figure 4.16. PCE concentrations at the WTP under the Original Schedule and Minimum Schedule I .......................................................... 131

Figure 4.17. Pumping rate and pumping capacity of well TT-26 under Minimum Schedule II .......................................................... 135

Figure 4.18. Comparison of PCE distribution in Layer 1 under the Original Schedule and Minimum Schedule II .......................................................... 137
Figure 4.19. Comparison of PCE distribution in Layer 3 under the Original Schedule and Minimum Schedule II ................................................................. 138

Figure 4.20. Comparison of PCE distribution in Layer 5 under the Original Schedule and Minimum Schedule II ................................................................. 139

Figure 4.21. Comparison of PCE distribution in Layer 1 under Minimum Schedule I and Minimum Schedule II ................................................................. 140

Figure 4.22. Comparison of PCE distribution in Layer 3 under Minimum Schedule I and Minimum Schedule II ................................................................. 141

Figure 4.23. Comparison of PCE distribution in Layer 5 under Minimum Schedule I and Minimum Schedule II ................................................................. 142

Figure 4.24. PCE concentrations at water-supply wells under the Original Schedule and Minimum Schedule II ........................................................................... 143

Figure 4.25. PCE concentrations at major water-supply wells under Minimum Schedule I and Minimum Schedule II during POI ............................................ 144

Figure 4.26. PCE concentrations at the WTP under the Original Schedule, Minimum Schedule I, and Minimum Schedule II ......................................................... 146

Figure 4.27. Percentage of pumping rate relative to its pumping capacity in well TT-26 under the Original and updated pumping schedules ........................................ 149

Figure 4.28. PCE concentrations at well TT-26 under the Original and updated pumping schedules ......................................................................................... 150

Figure 4.29. PCE concentrations at the WTP under the Original and updated pumping schedules ......................................................................................... 152

Figure 5.1. Illustration of the improved Monte Carlo simulation ................................................................. 160

Figure 5.2. Illustrations of spherical and exponential variogram models ................................................................. 164

Figure 5.3. Illustration of conditioning points for layer 1 ................................................................................. 166

Figure 5.4. Illustration of conditioning points for layer 3 ................................................................................. 167

Figure 5.5. Illustration of conditioning points for layer 5 ................................................................................. 167

Figure 5.6. Comparison of hydraulic conductivities in layer 1 between Camp Lejeune model and a FIELDGEN generation ................................................................. 168

Figure 5.7. Statistical results of $Q_{T-monthly}/Q_{T-yearly}$ ratios at Tarawa Terrace .................................... 171

Figure 5.8. Comparison of generated historical pumping demands to calibrated model 172
Figure 5.9. Relative change of CV vs. number of realizations for Scenario 1 .............. 177
Figure 5.10. Statistical results of PCE concentration at the WTP for Scenario 1 ......... 179
Figure 5.11. Frequency and cumulative probability of PCE concentration at the WTP exceeding the MCL for Scenario 1 ................................................................. 180
Figure 5.12. Probability of exceeding concentrations of PCE at the WTP for Scenario 1 .................................................................................................................. 181
Figure 5.13. Relative change of CV vs. number of realizations for Scenario 2 ........ 182
Figure 5.14. Statistical results of PCE concentration at the WTP for Scenario 2 .... 183
Figure 5.15. Frequency and cumulative probability of PCE concentration at the WTP exceeding the MCL for Scenario 2 ................................................................. 184
Figure 5.16. Probability of exceeding concentrations of PCE at the WTP for Scenario 2 .................................................................................................................. 185
Figure 5.17. Comparison of mean PCE concentrations at the WTP for different scenarios .................................................................................................................. 186
Figure 5.18. Comparison of $Q_{TT-26}/Q_{CTT-26}$ for different scenarios ............... 188
Figure 5.19. Comparison of mean values of $Q_{TT-26}/Q_{CTT-26}$ for different scenarios ...... 189
Figure 5.20. Comparison of probabilities of exceeding concentrations of PCE at the WTP for different scenarios .......................................................................... 190

Figure 6.1. Illustration of Pareto dominance ......................................................... 196
Figure 6.2. Flowchart of PDCRI .......................................................................... 197
Figure 6.3. The candidate well locations, contaminant source, hydraulic conductivity and initial head distributions for the example problem ......................... 200
Figure 6.4. The cumulative probability distributions for the earliest MCL arrival times and a theoretical normal distribution .......................................................... 202
Figure 6.5. Criticalness Indexes vs. reliabilities of realizations used in PDCRI .......... 204
Figure 6.6. Number of realizations with CI values greater than 0.90 and 0.95 for PDCRI applications with various numbers of realizations ........................................ 205
Figure 6.7. Cumulative probabilities of MCL arrival for critical realizations under the Maximum Schedule ..................................................................................... 210
Figure 6.8. Cumulative probabilities of MCL arrival for critical realizations under Minimum Schedule I. .............................. 211
### LIST OF ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANN</td>
<td>Artificial neural network</td>
</tr>
<tr>
<td>ASAP</td>
<td>Adjoint sensitivity analysis procedure</td>
</tr>
<tr>
<td>ATSDR</td>
<td>Agency for Toxic Substances and Disease Registry</td>
</tr>
<tr>
<td>CI</td>
<td>Criticalness Index</td>
</tr>
<tr>
<td>DDP</td>
<td>Differential dynamic programming</td>
</tr>
<tr>
<td>DES</td>
<td>Derandomized evolution strategy</td>
</tr>
<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Method</td>
</tr>
<tr>
<td>FOSM</td>
<td>First-order second moment</td>
</tr>
<tr>
<td>FSAP</td>
<td>Forward sensitivity analysis procedure</td>
</tr>
<tr>
<td>FTL</td>
<td>Flow-transport link</td>
</tr>
<tr>
<td>GA</td>
<td>Genetic algorithm</td>
</tr>
<tr>
<td>GSLIB</td>
<td>Geostatistical Software Library</td>
</tr>
<tr>
<td>IG</td>
<td>Improved Gradient</td>
</tr>
<tr>
<td>LA</td>
<td>Linear approximator</td>
</tr>
<tr>
<td>LP</td>
<td>Linear Programming</td>
</tr>
<tr>
<td>MCS</td>
<td>Monte Carlo simulation</td>
</tr>
<tr>
<td>MCL</td>
<td>Maximum Contaminant Level</td>
</tr>
<tr>
<td>NLP</td>
<td>Nonlinear Programming</td>
</tr>
<tr>
<td>PCE</td>
<td>Tetrachloroethylene</td>
</tr>
<tr>
<td>PDCRI</td>
<td>Pareto Dominance based Critical Realization Identification</td>
</tr>
<tr>
<td>POI</td>
<td>Period of interest</td>
</tr>
<tr>
<td>Acronym</td>
<td>Definition</td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
</tr>
<tr>
<td>PSOpS</td>
<td>Pumping Schedule Optimization System</td>
</tr>
<tr>
<td>QNDDP</td>
<td>Differential dynamic programming with quasi-Newton approximations</td>
</tr>
<tr>
<td>RAA</td>
<td>Rank-and-Assign</td>
</tr>
<tr>
<td>RR</td>
<td>Refreshment rate</td>
</tr>
<tr>
<td>SA</td>
<td>Simulated annealing</td>
</tr>
<tr>
<td>SALQR</td>
<td>Successive approximation linear quadratic regulator</td>
</tr>
<tr>
<td>S/O</td>
<td>Simulation/Optimization</td>
</tr>
<tr>
<td>SP</td>
<td>Stress period</td>
</tr>
<tr>
<td>TS</td>
<td>Tabu search</td>
</tr>
<tr>
<td>VOC</td>
<td>Volatile Organic Compound</td>
</tr>
<tr>
<td>WDS</td>
<td>Water Distribution System</td>
</tr>
<tr>
<td>WTP</td>
<td>Water Treatment Plant</td>
</tr>
</tbody>
</table>
SUMMARY

Health scientists often rely on simulation models to reconstruct groundwater contaminant exposure data for retrospective epidemiologic studies. Due to the nature of historical reconstruction process, there are inevitably uncertainties associated with the input data and, therefore, with the final results of the simulation models, potentially adversely impacting related epidemiologic investigations. This study examines the uncertainties associated with the historically reconstructed contaminant fate and transport simulations for an epidemiologic study conducted at U.S. Marine Corps Base Camp Lejeune, North Carolina. To achieve an efficient uncertainty analysis, sensitivity analysis was first conducted to identify the critical uncertain variables, which were then adopted in the uncertainty analysis using an improved Monte Carlo simulation (MCS) method. Particularly, uncertainties associated with the historical contaminant arrival time were evaluated. To quantify the uncertainties in an efficient manner, a procedure identified as Pumping Schedule Optimization System (PSOpS) was developed to obtain the extreme (i.e., earliest and latest) contaminant arrival times caused by pumping schedule variations. Two improved nonlinear programming methods – Rank-and-Assign (RAA) and Improved Gradient (IG) – are used in PSOpS to provide computational efficiency. Furthermore, a quantitative procedure named Pareto Dominance based Critical Realization Identification (PDCRI) was developed to screen out critical realizations for contaminant transport in subsurface system, so that the extreme contaminant arrival times under multi-parameter uncertainties could be evaluated efficiently.
CHAPTER 1
INTRODUCTION

1.1 Background

Groundwater is an invaluable natural resource that supplies a large portion of drinking water for human beings. Therefore, groundwater management problems, including groundwater quantity and groundwater quality management problems are always topics of great interest to researchers specializing in this field. In the past few decades, human activities such as agriculture, industry, and waste disposal have caused serious contamination of the groundwater system. The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA, also known as Superfund) of 1980 has led to the discovery of contaminated sites of groundwater and soil across the United States. The Environmental Protection Agency (EPA) estimated that the Superfund National Priorities List (NPL) could grow to more than 2,000 sites from the original 400 sites [NRC, 1999].

Groundwater contamination problems have led to intensive studies of contaminant fate and transport in the groundwater system. The transport of contaminants in a groundwater system is a very complicated process that can be affected by numerous hydrologic and hydrogeologic factors, physical and chemical properties of the porous media and the contaminants. Among these factors, pumping and/or injection activity in an aquifer plays an important role. The pumping and/or injection from wells (i.e., “pumping schedule”) can change the transport pathway of the contaminant in a subsurface system by influencing the advective transport parameters, and therefore, they
are very effective means through which we can impose control on the groundwater system. This property of pumping and injection has been utilized in engineering for controlled remediation of contaminated aquifer systems.

This study focuses on evaluating the change in the contaminant fate and transport process for a complex field-scale subsurface system that may be caused by the variation of the pumping schedule, as well as other variables such as hydrogeologic parameters and contaminant properties.

1.2 Motivation and Objective

Contaminated groundwater may cause serious human health problems. In particular, when contaminated groundwater serves as a source of the drinking water supply of a community, the users will be exposed to contaminants through their daily activities such as drinking and bathing. An epidemiologic study is a method used by health scientists to reveal the relationships between exposure to environmental contaminants and human health effects. However, epidemiologic studies are often retrospective and there is only limited quantitative historical information to conduct an exposure assessment. One method to improve the quality of retrospective epidemiologic studies is historical reconstruction and simulation analyses [Maslia et al., 2003; Nieuwenhuijsen et al., 2006]. When conducting environmental health studies associated with groundwater contaminants, researchers rely on groundwater flow and contaminant fate and transport models for reconstructing historical exposures to contaminants.

In assessing human exposure to groundwater contaminants, the key factors include the reliable estimate of historical contaminant concentration and the arrival time (i.e., the time for the contaminant concentration to exceed a specified level during a
contamination event) at the exposure point. During an historical reconstruction, the input parameters for flow and transport models are deterministic. Although the parameters are often calibrated by using measured site data, owing to the heterogeneous nature of the hydrogeologic parameters, a “true” mathematical description of a real-world site is extremely hard, if not impossible. Therefore, there are always uncertainties associated with the simulation results, which will significantly impact the accuracy and reliability of the related epidemiologic investigations.

Evaluation of uncertainties residing in the historically reconstructed exposure data can provide invaluable supportive information for the associated epidemiologic study. However, simulation models constructed for epidemiologic studies are often field-scale complex models, and the related uncertainty analysis can be computationally intensive. To conduct the uncertainty analysis in an efficient manner, several procedures were developed in this study. The efficiencies and reliabilities of these procedures were demonstrated using an epidemiologic study conducted at Marine Corps Base Camp Lejeune, North Carolina.

Historically, the Tarawa Terrace water distribution system (WDS) has supplied drinking water to the family housing at U.S. Marine Corps Base Camp Lejeune, North Carolina. It was detected that the WDS was contaminated with volatile organic compounds (VOCs), mostly with Tetrachloroethylene (PCE) [Maslia et al., 2007b]. Health issues such as specific birth defects and childhood cancers have been reported to occur in children born at the base. Therefore, the Agency for Toxic Substances and Disease Registry (ATSDR), U.S. Department of Health and Human Services, is conducting an epidemiologic study at this site to determine if exposure to contaminated
drinking water is related to birth defects and childhood cancer in children born to women who lived on base during the period 1968 – 1985 [Maslia et al., 2007b].

Due to the limited exposure data available for the period of interest (POI, January 1968 – December 1985), historical reconstruction method has been applied to simulate contaminant concentrations at the Tarawa Terrace water treatment plant (WTP), which supplied water to the Tarawa Terrace WDS. Data utilized include groundwater pumpage, well capacities and periods of operation, contaminant source location and release data, and contaminant concentrations at pumping wells located in Tarawa Terrace area [Maslia et al., 2007a].

In this study, uncertainties associated with the historical reconstructed PCE concentration and the maximum contaminant level (MCL, 5 ppb for PCE) arrival time at the Tarawa Terrace WTP were evaluated. Particularly, the changes of PCE concentrations and MCL arrival times caused by pumping schedule variations were investigated using a Pumping Schedule Optimization System (PSOpS) employing a Simulation/Optimization (S/O) approach. Furthermore, a Pareto Dominance based Critical Realization Identification procedure was developed to be used together with PSOpS to quantify the extreme variations in contaminant transport caused by multiple uncertain parameters.

1.3 Organization of the Thesis

A literature review of the research topics relevant to this study is provided in Chapter 2. These topics include application of S/O approach to optimization of groundwater remediation strategies, groundwater flow and contaminant fate-and-
transport simulation models, optimization techniques used in the S/O approach, optimizations under uncertainty, and sensitivity and uncertainty analyses.

In Chapter 3, numerical simulations of the groundwater flow and contaminant fate and transport in Tarawa Terrace area of U.S. Marine Corps Camp Lejeune, which were conducted by ATSDR, are briefly introduced. After the uncertain variables in these simulation models are identified, sensitivity analyses to these uncertain variables are conducted to identify the most critical uncertain variables for the followed uncertainty analysis.

Prior to the uncertainty analysis, the effect of pumping schedule variation on PCE concentrations and MCL arrival times at the Tarawa Terrace WTP is evaluated by applying the newly developed Pumping Schedule Optimization System (PSOpS) in Chapter 4.

In Chapter 5, an improved uncertainty analysis procedure for field-scale systems is developed by using Monte Carlo simulation (MCS). Uncertainty analyses with and without pumping schedule in consideration are compared to demonstrate the effect of pumping schedule variation on contaminant transport.

Extreme variations of PCE MCL arrival times at the WTP that are caused by multiple uncertain variables are evaluated in Chapter 6, which is followed by the conclusions in Chapter 7. To accomplish the evaluation in a timely manner, a procedure identified as Pareto Dominance based Critical Realization Identification (PDCRI) was proposed to screen out a few critical realizations from a large set of realizations. Applications of PSOpS to these critical realizations can yield extreme contaminant arrival times efficiently while maintaining a high reliability.
CHAPTER 2

LITERATURE REVIEW

2.1 S/O Approach and Its Application to Groundwater Remediation Problems

Groundwater serves as an important source of drinking water. Contamination of groundwater by various industrial and waste disposal activities has become a serious environment problem. During the past two decades, much attention has been paid to groundwater remediation problems. Due to the high cost associated with the remediation process and the potential cost reduction by optimization, the optimization of groundwater remediation strategies has been widely studied [Cunha, 2002; Das and Datta, 2001; Freeze and Gorelick, 1999; Gorelick, 1983; Wagner, 1995].

Due to the complexity of groundwater flow and contaminant fate and transport, for a complex real-world flow and transport problem, analytical solutions are not available for most of the cases [Cunha, 2002]. Therefore, mathematical optimization techniques have been combined with aquifer simulation models to address groundwater quality management problems [Wagner, 1995]. In this thesis, our interest is limited to the applications of S/O to the optimal design of the pump-and-treat systems.

A typical S/O application includes four parts: flow and transport models, an optimization formulation, the incorporation of simulation models into the optimization problem, and an appropriate optimization technique that is used to solve the problem. Flow and transport models are essential because they can predict the system response to specified management strategies. The optimization formulation is used to specify the management objectives, such as total costs minimization or withdrawn mass
maximization, and constraints on hydraulic heads, drawdowns, pumping capacities, head gradients, and so forth. The incorporation of simulation model integrates the simulation models into the optimization process by embedding the models into the optimization formulation, direct coupling, or incorporation of simulation models through a response function. Considering the management objectives and constraints, an appropriate optimization method is then selected to identify the best remediation strategy in a cost-effective manner [Wagner, 1995].

Extensive reviews about the S/O applications to design of groundwater remediation system can be found in works by Gorelick [1983], Wagner [1995], Freeze and Gorelick [1999], Das and Datta [2001], and Cunha [2002].

2.1.1 Aquifer Simulation Models

A prerequisite for applying S/O to a site study is the development of calibrated flow and transport models for the target site. Groundwater flow and contaminant fate-and-transport in a groundwater system are governed by the following two equations [Charbeneau, 2000]:

\[ S_s \frac{\partial h}{\partial t} + \nabla \cdot q = W , \]  
(2.1)

and

\[ \frac{\partial m}{\partial t} + \nabla \cdot J = S . \]  
(2.2)

Equation (2.1) is the continuity equation of groundwater flow. In the equation, \( S_s \) is the specific storage of the porous medium (L\(^{-1}\)); \( h \) is the piezometric head (L); \( t \) is time (T); \( q \) is the Darcy velocity vector (LT\(^{-1}\)); and \( W \) is a volumetric flux per unit volume that represents sources and/or sinks at the site (T\(^{-1}\)).
Equation (2.2) is the continuity equation governing the contaminant transport in the groundwater system. In equation (2.2), $m$ is the contaminant bulk concentration (ML$^{-3}$); $t$ is time (T); $J$ is the general mass flux vector composed of advective and dispersive fluxes (ML$^{-2}$T$^{-1}$); and $S$ is the strength of the sinks and sources, which also includes the reaction terms of the contaminant (ML$^{-3}$T$^{-1}$).

Due to the complexity of these governing equations, especially for field-scale groundwater systems, they cannot be solved analytically. Traditionally, these governing equations are usually solved numerically by using the finite difference method (FDM) or the finite element method (FEM). Various simulations codes have been developed to solve either one or both of these two equations. The most frequently used codes include MODFLOW [McDonald and Harbaugh, 1984], which solves three-dimensional groundwater flow using FDM, and MT3DMS [Zheng and Wang, 1999a], which is a three-dimensional contaminant transport simulator based on FDM. These two codes have been applied to several S/O applications [e.g., Huang and Mayer, 1997; Maskey et al., 2002; Sawyer and Lin, 1998; Wang and Zheng, 1997, 1998a]. More detailed information regarding these two codes can be found in Section 2.2.

Other simulation codes that have been applied to groundwater remediation design include ISOQUAD [Pinder, 1979], an implicit finite element groundwater flow and transport model for a confined two-dimensional aquifer [e.g., Culver and Shoemaker, 1992, 1993; Culver and Shenk, 1998], and SUTRA [Voss, 1984], a finite element 2D or 3D saturated-unsaturated groundwater flow and contaminant transport model [e.g., Bear and Sun, 1998; Gorelick et al., 1984; Wagner and Gorelick, 1987].
2.1.2 Formulation of Optimization Problems

For the optimal design of a groundwater remediation system, an optimization problem should be carefully formulated to reflect the management objectives and constraints. Formulation of the optimization problem can affect the selection of appropriate optimization methods, and vice versa.

In these problems, three types of management objectives can be identified based on the remediation goals selected. Maximization of contaminant mass removal [e.g., Zheng and Wang, 2002] and minimization of cleanup time [e.g., Maskey et al., 2002] are often used as objective functions in aquifer restoration problems, while total costs minimization [e.g., Ahlfeld et al., 1995; Guan and Aral, 1999; Ratzlaff et al., 1992] has been used for both aquifer restoration and contaminant plume containment problems. In the literature, cost functions are more frequently adopted as the objective functions. A cost function usually consists of two parts: operation costs and capital costs. Operation costs typically include pumping cost and treatment cost, while capital costs consist of well installation costs, treatment facility costs, and management costs. Sometimes, a third part, penalty cost, is also included in the objective function to reflect the cost caused by failures to meet the design constraints, or to convert the problem to a non-constrained one.

Formulation of objective function limits the optimization method to be used. For example, traditional nonlinear programming techniques require the objective function to be continuous and differentiable. Therefore, these methods can be applied to problems with continuous objective functions only, such as operational cost functions. Addition of capital costs to objective functions makes them neither differentiable nor continuous.
Problems with this type of objective functions have found solutions successfully using heuristic optimization methods [Cunha, 2002].

Decision variables are the engineered features to be optimized. For a pump-and-treat system, the decision variables can be the number of wells to be installed, well locations, and pumping and/or injection rates in the wells. One or more of these variables can be put into a formulation. According to the optimization techniques applied, these variables can be formulated into either continuous or discrete ones. These variables can be also defined to be invariant, or sometimes time-varying for more flexible and cost-efficient remediation strategies [Freeze and Gorelick, 1999].

Constraints in the optimization formulations reflect the final management goals, and other natural or management restrictions regarding the remediation process. Mulligan and Ahlfeld [1999] grouped optimal remediation designs into three categories: transport-based concentration control, flow-based hydraulic control, and particle tracking-based advective control. For concentration control designs, the constraints are usually the maximum concentrations at control points [e.g., Guan and Aral, 1999]. The constraints for hydraulic control designs include predefined head gradient, head difference, or velocities at specified points [e.g., Ratzlaff et al., 1992]. Advective control designs required all contaminant particles to terminate at pumping wells [e.g., Bayer and Finkel, 2004; Mulligan and Ahlfeld, 1999]. Other natural and management restrictions impose constraints on pumping capacities, treatment capacities, drawdown limits, and etc.

2.1.3 Incorporation of Simulation Models

With the optimization problem properly formulated according to management objectives and constraints, simulation models need to be incorporated into the S/O
process. As stated by Gorelick et al. [1984], three means exist to link the simulation models to the optimization process: embedding, direct coupling, and response matrix.

Sometimes the finite difference flow and contaminant transport equations (2.1) and (2.2) are embedded into the optimization problems as constraints [e.g., Guan and Aral, 1999], which means that the equations are solved within the optimization process. More often, when groundwater flow and contaminant transport in a complex system are involved in the optimization, existing simulation codes such as MODFLOW and MT3DMS are directly coupled into the optimization model to provide system responses [e.g., Wang and Zheng, 1997].

Optimization using embedding and direct coupling are computationally intensive because that during the optimization process the flow and transport models are often run repeatedly till convergence. In fact, for the optimal remediation design problems, most of the computational sources are applied to the numerical simulations of flow and transport. A major objective of applying and improving various optimization methods is to reduce the computational requirement associated with the simulations.

To alleviate the computational burden associated with the numerical simulations, in some applications, a response matrix approach has been used in place of simulation models to provide the hydraulic response due to specific pumping strategies [e.g., Zheng and Wang, 1999b]. However, since this approach is based on the principle of superposition, it can be only applied to linear systems [Freeze and Gorelick, 1999].

**2.1.4 Optimization Techniques**

Prior to the application of S/O approach, the remediation strategy was typically designed by the so called “trial-and-error” method. Using this approach remediation
strategies are evaluated, compared, and then improved gradually. The drawbacks of the trial-and-error method are apparent. First, this method can be very time consuming. Second, by using this method, no optimal solutions can be guaranteed.

Linear programming (LP) was first applied to deterministic optimization of groundwater remediation policies [e.g., Atwood and Gorelick, 1985]. While it has advantages, such as simplicity, the application of LP to optimal remediation design remains limited due to the fact that most real-world flow and transport are nonlinear. Therefore, nonlinear optimization techniques were introduced. Owing to the heterogeneous nature of the groundwater systems, optimization under system uncertainties is also attracting more research interest. As is stated by Gorelick [1997], the trend of groundwater management problems changes from linear and deterministic to nonlinear and stochastic.

Optimization techniques that have been applied to optimal remediation design problems can be put into two categories: traditional mathematical programming methods and heuristic methods [Cunha, 2002]. Compared with the traditional methods, the heuristic methods have a shorter history of application. They have gained importance because of their ability to overcome some of the formulation limitations caused by classical methods. The traditional methods include linear programming (LP), nonlinear programming (NLP), control theory algorithms, and successive approximation method. The heuristic methods include genetic algorithms (GA), simulated annealing (SA), tabu search (TS), and derandomized evolution strategy (DES). Sometimes, two or more optimization methods are applied together to take advantages of the individual characteristics of each method.
A more detailed explanations and applications regarding various optimization methods can be found in Section 2.3. The optimal design of groundwater remediation policies under uncertainty is extensively reviewed in section 2.4.

2.2 MODFLOW and MT3DMS

In the S/O approach applied to groundwater quality management problems, numerical simulation models are used to answer the question of “what if,” i.e., to provide the system response, such as heads and concentrations, to the input boundary conditions or scenarios. Various flow and transport simulation codes based on either FDM or FEM exist in the literature. Among these codes, MODFLOW [McDonald and Harbaugh, 1984] and MT3DMS [Zheng and Wang, 1999a] are used frequently. These two codes also serve as flow and transport simulators in this study.

2.2.1 MODFLOW

MODFLOW is a computer program that was designed to solve the three-dimensional groundwater flow equation by using FDM [McDonald and Harbaugh, 1988] for both steady state and transient flow applications:

\[
\frac{\partial}{\partial x} (K_{xx} \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y} (K_{yy} \frac{\partial h}{\partial y}) + \frac{\partial}{\partial z} (K_{zz} \frac{\partial h}{\partial z}) + W = S_s \frac{\partial h}{\partial t},
\]

in which \( K_{xx}, K_{yy}, \) and \( K_{zz} \) are hydraulic conductivity values along the \( x-, y-, \) and \( z- \) coordinate axis directions (L/T); \( h \) is the piezometric head (L); \( W \) is a volumetric flux per unit volume that represents sources and/or sinks at the site (T\(^{-1}\)); \( S_s \) is the specific storage of the porous medium (L\(^{-1}\)); \( t \) is time (T); and \( x, y, z \) are the Cartesian coordinate directions (L).
MODFLOW was originally developed by McDonald and Harbaugh [1984]. Since then it has been modified for numerous times, and several different versions exist in the literature. The second version is identified as MODFLOW-88 [McDonald and Harbaugh, 1988]. The third version is identified as MODFLOW-96 [Harbaugh and McDonald, 1996a, b]. The latest version, which is used in this study, is identified as MODFLOW-2000 [Harbaugh et al., 2000]. Since its inception, the following authors – Prudic [1989], Hill [1990], Leake and Prudic [1991], Goode and Appel [1992], Harbaugh [1992], McDonald et al. [1992], Hsieh and Freckleton [1993], Leake et al. [1994], Fenske et al. [1996], [Leake and Lilly [1997], and Hill et al. [2000] – have made several improvements to MODFLOW.

In MODFLOW simulations, a fundamental component of the time discretization data is the “time step.” A group of time steps are identified as a “stress period” [Harbaugh et al., 2000]. Within a stress period, the time dependent variables, such as the groundwater pumping rates of pumping wells, are constant. The basic spatial simulation unit used in the finite-difference calculations is called a “finite-difference cell” or “cell.”

The input data for the MODFLOW simulation can be divided into two categories: (i) “global process input” data file and, (ii) “groundwater flow process input” data file. Global process input files contain basic information which is applied to the whole simulation. As for the groundwater flow process input files, a group of related input data are put together into a file as the input for a specific “package.” Tens of packages exist in the MODFLOW codes. Here only input files related to this study are introduced.

There are two global process files used in the study:

i.  **File type:** NAM
File contents: The name information of each file used in the simulation;

ii. File type: DIS

File contents: Basic space and time discretization information.

The following nine groundwater flow process files are also used in the study:

i. File type: BAS6

Package: Basic Package

File contents: Boundary conditions and initial head distribution;

ii. File type: BCF6

Package: Block-Centered Flow Package

File contents: Hydraulic characteristics regarding groundwater flow such as hydraulic conductivities and storage coefficients;

iii. File type: DRN

Package: Drain Package

File contents: Drain cells information;

iv. File type: GHB

Package: General-Head Boundary Package

File contents: General-head cells information;

v. File type: OC

Package: Output Control Option

File contents: Output specifications;

vi. File type: PCG

Package: Preconditioned Conjugate-Gradient Package

File contents: Solver parameters;
vii. **File type**: RCH

**Package**: Recharge Package

**File contents**: Recharge information;

viii. **File type**: LMT6

**Package**: Link-MT3DMS Package

**File contents**: Specifications for the flow-transport link (FTL) file;

ix. **File type**: WEL

**Package**: Well Package

**File contents**: Well information such as well locations and pumping rates.

### 2.2.2 MT3DMS

MT3DMS is a modular three-dimensional multi-species transport model that can be used in the simulation of advective, dispersive, and reactive transport of contaminants in groundwater flow systems [Zheng et al., 2001]. The governing equation used in the MT3DMS simulation model can be given as:

\[
\frac{\partial (\theta C^k)}{\partial t} = \frac{\partial}{\partial x_j} (\theta D_{ij} \frac{\partial C^k}{\partial x_j}) - \frac{\partial}{\partial x_i} (\theta v_i C^k) + q_s C_s^k + \sum R_n, \tag{2.4}
\]

where \( \theta \) is the porosity of subsurface system; \( C^k \) is the concentration of species \( k \) in aqueous phase (ML\(^{-3}\)); \( t \) is time (T); \( x_i \) and \( x_j \) are the distances along the three-dimensional Cartesian coordinate axis directions (L); \( D_{ij} \) is the dispersion coefficient (L\(^2\)T\(^{-1}\)); \( v \) is pore velocity (LT\(^{-1}\)); \( q_s \) is the flow rate per unit volume of aquifer representing sinks and sources (T\(^{-1}\)); \( C_s^k \) is the concentration of species \( k \) in sink or source flux (ML\(^{-3}\)); and \( \sum R_n \) is the chemical reaction term (ML\(^{-3}\)T\(^{-1}\)).
Prior to an MT3DMS simulation, an MODFLOW simulation is always required to provide necessary groundwater flow information through a FTL file. Similar to the input files of MODFLOW, the input files of MT3DMS include one name file and some other input files used for various packages.

i. **File type**: NAM

*File contents*: The name information of each file used in the simulation;

ii. **File type**: BTN

*Package*: Basic Transport Package

*File contents*: Basic model information required for the contaminant simulation including space and time discretization, aquifer properties regarding contaminant transport such as porosity, contaminant properties and initial condition;

iii. **File type**: ADV

*Package*: Advection Package

*File contents*: Advective transport simulation variables;

iv. **File type**: DSP

*Package*: Dispersion Package

*File contents*: Contaminant dispersion regarded properties;

v. **File type**: SSM

*Package*: Sink and Source Mixing Package

*File contents*: Sink and source terms used in contaminant transport;

vi. **File type**: RCT

*Package*: Chemical Reaction Package
File contents: Parameters regarding the chemical reactions of contaminant such as reaction rates;

vii. File type: GCG

Package: Generalized Conjugate-Gradient Solver Package

File contents: Solver parameters;

viii. File type: FTL

Package: Flow-Transport Link Package

File contents: The groundwater flow related information.

2.3 Optimization Methods Applied to Groundwater Study

In the past two decades, application of S/O approach has provided a framework to replace the traditional trial-and-error method for the optimization of remediation strategies. A variety of optimization methods have been used for groundwater quality management problems. It has been demonstrated that the S/O approach is more advantageous in finding cost-effective remediation strategies. In this section, various optimization techniques found in the literature are reviewed under three major groups: classical mathematical programming methods, heuristic methods, and hybrid methods.

2.3.1 Classical Mathematical Programming Methods

The application of optimization methods to groundwater management problems started with classical mathematical programming methods. This is easy to understand since these methods have been widely applied to other fields such as applied physics and operations research before their application to groundwater area and lots of experience exists towards the application of these methods.
Various classical mathematical methods have been applied to the groundwater quality management problems, such as linear programming (LP) [Atwood and Gorelick, 1985], nonlinear programming (NLP) [Ahlfeld et al., 1988a, b; Bear and Sun, 1998; Gorelick et al., 1984; Wagner and Gorelick, 1987; Wang and Ahlfeld, 1994], control theory algorithms [Chang et al., 1992; Culver and Shoemaker, 1992, 1993, 1997; Culver and Shenk, 1998], successive approximation methods [Karatzas and Pinder, 1993; 1996], and more.

For most classical mathematical optimization methods, one major disadvantage is that the objective function is theoretically assumed to be continuous and twice differentiable [Dougherty and Marryott, 1991]. While the capital costs have been proved to have significant impacts on the optimal remediation policies [Culver and Shoemaker, 1997; Culver and Shenk, 1998; Hsiao and Chang, 2002], using traditional optimization algorithms to find optimal solutions for remediation problems considering capital costs remains challenging due to the discontinuous nature of the capital cost function in the objective function.

Another drawback of conventional optimization techniques is that the solution cannot be guaranteed to be globally optimal due to the nonconvex nature of the optimization problems, which is typically for groundwater flow and contaminant transport problems [Ahlfeld and Palumbo, 1996].

2.3.1.1 Linear Programming

Linear programming (LP) was the first optimization technique applied to the S/O solution of groundwater management problems [Gorelick, 1983]. The primary advantages of LP include that the solution using simplex algorithm is relatively easy to
obtain, and that the solution is guaranteed to be the global optimum if a solution exists
[Ahlfeld and Heidari, 1994].

Atwood and Gorelick [1985] applied LP to optimize a groundwater remediation system using hydraulic gradient control method. In their approach, a two-stage planning procedure was adopted. In the first stage, the approximated contaminant plume boundary as a function of time was determined. In the second stage, LP was used to find the best well locations and pumping/injection rates to minimize the pumping cost while satisfying the hydraulic gradient requirements. A response matrix was used to reflect the gradient changes at gradient check locations caused by variation of pumping/injection rates in different well locations. In their study, the unconfined aquifer was approximated to be confined to permit the use of a linear response function technique based on the principle of superposition.

Application of the response matrix with linearity assumption avoids the requirement for analytical calculation of derivatives and thus saves computational sources. However, the principal of superposition can be only applied to linear systems. As it is well known, most real-world contaminant transport problems are nonlinear. Therefore, although many cases exist in the literature regarding the application of LP to groundwater quantity management problems, application of LP to groundwater quality management problems remains very limited and can be only applied to physical containment of contaminant plume, in which no contaminant concentration is involved.

2.3.1.2 Nonlinear Programming

Groundwater quality management problems with contaminant concentration involved are typically nonlinear. To handle the important nonlinearities in the
optimization of groundwater remediation schemes, application of nonlinear programming (NLP) methods has been proposed.

In the work of Gorelick et al. [1984], a nonlinear programming package called “MINOS” [Murtagh and Saunders, 1978, 1982] was used together with a finite element flow and transport simulator “SUTRA” [Voss, 1984] to find the optimal aquifer reclamation design. MINOS is a well-known nonlinear optimization program for solving nonlinearly constrained problems using the gradient method combined with a projected Lagrangian function.

The basic idea of MINOS is to define a sub-problem with only linear constraints by using linearizations of the nonlinear constraints and approximations of the Lagrange multipliers. In their study, MINOS was used to minimize the total pumping rates while satisfying the concentration and drawdown constraints. MINOS was also used by Ahlfield et al. [1988a; 1988b] and Wang and Ahlfield [1994] to minimize the contaminant mass left in the aquifer and the pumping cost for optimal groundwater remediation designs.

Bear and Sun [1998] proposed an optimization formulation for a multi-stage groundwater remediation design. Their formulation is a two-level hierarchical optimization model. At the upper level, the number of pumping and injection wells is optimized for minimal cost, while at the basic level, the well locations and pumping/injection rates are optimized for maximum solute mass removal. In their study, an NLP method, the steepest decent method was used.

The steepest descent method is a gradient-based method [Press et al., 1989]. To solve a minimization problem by using this method, from a starting point, the downhill gradient at that point is calculated, and a minimization point along the gradient direction
is found. From that point, the downhill gradient is calculated, and another point along the gradient direction is found. By following this gradient direction on the objective function, an optimal solution that meets termination criterion can be found. The problem with the Steepest Gradient method is that the iterated solutions may move into a direction of reversed gradient paths because the gradient at a new point can be perpendicular to the previous gradient. This increases the computational burden and may lead to an inefficient method.

One drawback of the NLP methods is that since most of these methods are gradient-based, the objective functions of the optimization formulations need to be continuous and differentiable. Since the incorporation of capital costs of groundwater remediation into the objective function causes the function discontinuous and non-differentiable, this drawback limits the application of NLP methods to groundwater quality management problems with capital costs under consideration.

Another limitation of the NLP methods is that no global optimal solution can be guaranteed for a nonconvex problem. It has been demonstrated that the response of concentration to pumping can be nonconvex even for relatively simple cases [Ahlfeld and Palumbo, 1996]. Therefore, a global optimal solution cannot be guaranteed using the traditional NLPs [Dougherty and Marryott, 1991]. A solution to this issue is using numerous different solutions as the starting points of optimization. However, considering the heavy computational burden associated with the flow and transport simulations, this approach can be very computationally demanding.
Control Theory Algorithms

In some groundwater quality management studies, the pumping/injection rates and well locations are considered as time-independent decision variables. However, solute transport processes in aquifers are never steady [Bear and Sun, 1998]. Control theory algorithms have also been combined with numerical simulation models to obtain optimal dynamic decontamination strategies for groundwater quality management problems, which have been demonstrated to be more cost effective than other static policies [Chang et al., 1992; Culver and Shoemaker, 1992, 1993, 1997; Culver and Shenk, 1998]. Control theory algorithms were specially developed to handle dynamic systems. The advantage of such algorithms is that they can handle dynamic problems with multiple management periods with only a linear increase in computational resources, while for nonlinear programming methods, the computational demand will increase much more rapidly [Chang et al., 1992]. However, there are also disadvantages associated with these control theory algorithms. First, control theory algorithms typically require a problem to be convex to ensure a rapid convergence [Culver and Shenk, 1998]. Therefore, for a cost-minimization pump-and-treat problem, quite often only operation costs (i.e. treatment costs and pumping costs) are used as an approximation for total cost, while the capital costs, such as well installation costs and facility costs, can not be easily put into the problem formulation. Second, application of control theory algorithms requires an initial guess of pumping rates, which is called “nominal policy.” The selection of nominal policy can strongly influence the speed of convergence [Chang et al., 1992]. Finally, similar to other nonlinear programming methods, control theory algorithms can not guarantee a global optimal solution as well.
Chang et al. [1992] applied an optimal control algorithm called SALQR (successive approximation linear quadratic regulator) to obtain optimal time-varying pumping policies for a pump-and-treat problem. The SALQR technique is developed based on the DDP (differential dynamic programming). The original DDP algorithm is difficult to apply to groundwater quality management problems because the second derivatives of the transition equation are too complicated to compute. The distinction between the SALQR approximation method and the DDP is that the SALQR method omits the second derivatives by approximating the transition equation as a linear equation. In other words, if the transition equation is linear, then they are basically the same. The results indicate that dynamic pumping policies can be much more cost-effective than static ones. But in cases with slow contaminant movement, invariant policies may be good enough.

In the work by Chang et al. [1992] the pumping policies are changed by the simulated time step used in the simulation model. However, in a real-world case this is unlikely to happen. With this in mind, Culver and Shoemaker [1992] applied the SALQR with the concept of “management periods,” which are groups of simulation time steps during which the pumping policy remains constant. Their results indicate that application of management periods can reduce the total computational demand significantly, but the optimal costs will be increased as the number of management periods is reduced. The optimal policy will change significantly as the number of management periods changes as well.

From another aspect, Mansfield and Shoemaker [1999] extended the application of the SALQR method from confined aquifer problems to unconfined aquifer cases,
which are more complicated. In their work, exact derivative equations are compared with two computationally efficient approximations, the quasi-confined (QC) and head independent from previous (HIP) unconfined aquifer finite element derivative approximations. The two approximations are demonstrated to be very accurate and can be applied to simplify some unconfined aquifer optimization problems.

Different from the SALQR method, which sets the second order derivatives of the transition equations to be zero, QNDDP (differential dynamic programming with quasi-Newton approximations) uses a Broyden rank-one quasi-Newton technique to approximate the second derivatives of the groundwater quality model \cite{CulverShoemaker1993}. For complex and time-varying systems, QNDDP has been shown to converge more quickly than the SALQR method.

As discussed in the introduction, application of optimal control algorithms requires a convex objective function for rapid convergence. Therefore, difficulty exists for control theory algorithms to incorporate capital costs to the cost function, which will make the objective function nonconvex. \textit{Culver and Shoemaker} \cite{CulverShoemaker1997} developed a method to bring the facility capital cost into consideration using QNDDP. In their development, the facility capacity is defined to be a state variable, as opposed to a decision variable. It is also supposed that the capacity in the first management period is the maximum capacity. The optimization results indicate that capital costs may affect a dynamic management policy significantly. Further effort has been made to incorporate other capital costs into the objective function for control theory algorithms \cite{CulverShenk1998}. By using a more realistic cost function associated with a granular activated carbon treatment system, \textit{Culver and Shenk} \cite{CulverShenk1998} demonstrated that control theory
algorithms still have difficulties dealing with optimization problems with nonconvex objective functions. Therefore, further improvement on control theory algorithms is suggested.

2.3.1.4 Successive Approximation Method

Due to the difficulty of solving nonlinear optimization problems with discontinuous objective functions using the traditional gradient-based NLPs, in such formulations capital costs such as well installation costs are often neglected. However, capital costs can be an important factor for an optimal remediation design, especially for short-term remediation problems.

Karatzas and Pinder [1993] proposed the outer approximation method, which is a kind of successive approximation method, to solve the pump-and-treat problems with the capital cost considered, which is a concave minimization over a compact convex set of constraints. Outer approximation method was developed based on the fact that the minimum of a concave function over a compact set of constraints is always located at one extreme point of the set.

In the application of outer approximation method, initially the feasible region is relaxed to a simpler constraint set over which the objective function is minimized. If the optimal solution falls into the original feasible region, it is the global optimum. Otherwise part of the relaxed constraint set containing the infeasible solution will be cut off and the minimization takes place again. The process is repeated till the global minimum is found.

One limitation of the outer approximation method is that the constraint set must be convex. However, it is well known that the response of concentration to pumping is often nonconvex [Ahlfeld and Palumbo, 1996]. In the work of Karatzas and Finder
the outer approximation method was improved to work on optimization problems with nonconvex constraints.

One advantage of the outer approximation method is that for this method does not require the evaluation of derivatives of the objective function, which can potentially improve the computational efficiency. However, for the method to be applied, a concave objective function is always necessary.

### 2.3.2 Heuristic Optimization Methods

During recent years, more and more heuristic methods have been applied to groundwater quality management problems because of their appealing features. Heuristic methods are sometimes referred to as global optimization methods because of their ability to find global or near global optimal solution. Heuristic methods are also called gradient-free methods because of the fact that they identify the optimal solution by objective function evaluation instead of the gradient information. Therefore, heuristic methods don’t require the objective function to be differentiable or convex.

Most applications of heuristic optimization methods are on combinatorial optimization problems, in which decision variables are discrete. Instead of enumerating all possible solutions, in heuristic methods, the decision space is searched in a guided manner, which can reduce the computational demand of running flow and/or transport simulations significantly.

The three most popular heuristic methods are genetic algorithms (GAs), simulated annealing (SA), and tabu search (TS) [Reeves, 1996]. GAs have been applied by Rogers and Dowla [1994], McKinney and Lin [1994], Rogers et al. [1995], Huang and Mayer [1997], Guan and Aral [1999]; SA methods have been used by [Dougherty and Marryott
[1991], Kuo et al. [1992], Marryott et al. [1993], Rizzo and Dougherty [1996], Wang and Zheng [1998a], Skaggs et al. [2001], Rao et al. [2003]; TS methods have been used by Zheng and Wang [1999b].

Recently, application of another heuristic method, derandomized evolution strategy (DES), to the optimization of groundwater remediation strategies was introduced by Yoon and Shoemaker [1999] and Bayer and Finkel [2004].

Although heuristic methods are robust for solving problems with discrete and nonconvex objective functions, they have their own drawbacks. The major disadvantage is their huge computational demands because that a large number of simulation runs are needed to converge. As we all know, for groundwater quality management problems, the major computational burden comes from the flow and transport simulation. Therefore, the application of heuristic methods to large field-scale problems remains limited and further improvement is required.

2.3.2.1 Genetic Algorithms

Genetic algorithms (GAs) are heuristic global searching algorithms introduced by Holland [1975] to simulate the natural evolution process. Goldberg [1989] addressed a detailed introduction to the application of GA. According to Goldberg [1989], there are four major differences between GA and traditional mathematical methods: (1) the GA typically codes the decision variable set into a binary string; (2) the GA searches the optimal solution from a population of decision variables sets; (3) the GA requires no derivative information; and (4) the GA uses probabilistic search rules.

In a GA process, the solution is expressed as a string (chromosome). During the process, first an initial population is generated and the fitness (objective function value)
of each string is evaluated. Then, a mating pool is generated from the current population using several GA operations, such as crossover operation (two parent strings obtained from the mating pool exchange part of their strings to form two new child strings) and mutation operation (values at some points of some strings are changed randomly). After the generation of new population, the fitness of each new string is evaluated again. This evolutionary process leads to the fittest strings to remain and accumulate in the population. If the termination criterion is met, the process stops. Otherwise, the process will start again based on the new generation of population.

GA is probably the most widely applied heuristic method to the groundwater quality management problems. In most of the works, adjustments were made to the classical GA paradigm to find high-quality solutions [Espinoza and Minsker, 2006; Guan and Aral, 1999, 2004, 2005; Hilton and Culver, 2005; Huang and Mayer, 1997; McKinney and Lin, 1994; Reed et al., 2000, 2003; Ritzel et al., 1994; Rogers and Dowla, 1994; Rogers et al., 1995; Smalley et al., 2000; Wang and Zheng, 1997].

McKinney and Lin [1994] compared optimizations of groundwater management problems using GA with other classical mathematical methods, such as linear, nonlinear, and dynamic programming. They demonstrated that GA has the ability to obtain globally (or near globally) optimal solutions. The optimal results obtained by GA are as good as, if no better than, those obtained by other traditional methods.

Ritzel et al. [1994] formulated two variations of GA to solve multiple objective groundwater remediation problems: a vector-evaluated GA (VEGA) and a Pareto GA. The two objectives under consideration are reliability maximization and cost
minimization, and a trade-off curve regarding these two variables can be generated by these multiple objective GAs for decision support.

Different from previous works, in which the well locations were pre-assigned, in the work by Huang and Mayer [1997] both the pumping rates and well locations are used as decision variables. Their results indicate that dynamic well locations and pumping rates are more cost-effective that fixed-well formulations, and the optimization problem is more sensitive to well locations than to pumping rates. The optimization of time-varying management strategies using GA was also studied by Wang and Zheng [1997]. To incorporate well locations into decision variables, Guan and Aral [1999] proposed a progressive genetic algorithm (PGA) to solve a pump and treat system in which the well locations and pumping rates are both defined as continuous decision variables.

Compared with traditional gradient-based methods, GA methods do not require the objective function to be continuous, convex, or differentiable. They also have advantages, such as robustness and easy implementation. However, owing to the large number of forward simulation runs needed to converge, they are very computationally demanding, especially for large size problems with a large mating pool. Therefore, application of GA methods to field-scale problems remains very limited [Zheng and Wang, 2002].

2.3.2.2 Simulated Annealing

The simulated annealing (SA) was developed by analogy to the statistical mechanics of annealing of solids. The basic ideas of SA were first introduced by Metropolis et al. [1953]. In their work, an algorithm was used to simulate the annealing process, during which the energy of a system is slowly decreased till the steady state (the
minimum energy state). Kirkpatrick et al. [1983] suggested the application of this simulation to solution of optimization problems. Ever since then, SA has been applied to large scale optimization problems in various fields.

SA is similar to the neighborhood search method, which searches for optimal solution by moving from one solution to another one in its neighborhood. The disadvantage of a neighborhood search method is that the solution can be easily trapped at local optimum. SA overcomes this drawback by allowing randomly moves to inferior solutions under some probabilistic control [Reeves, 1996].

Dougherty and Marryott [1991] used four highly idealized combinatorial problems to demonstrate the application of SA to the optimization of groundwater management problems. They have been able to demonstrate that SA can find good solutions to problems with highly variable objective functions. However, in their work, the pumping rates were simulated discretely but not continuously, which might not yield the optimal solution. The application of SA was extended to a two dimensional field-scale problem by Marryott et al. [1993]. These works indicate that the heavy computational burden from the flow and transport simulations in SA optimization still needs to be circumvented.

Kuo et al. [1992] presented the application of SA to the design of groundwater remediation system using a pump-and-treat strategy. In their formulation, the well installation costs were incorporated into the objective function, which caused the function to be non-differentiable.

SA has also been applied to optimize time-varying remediation polices for groundwater remediation problems [Rizzo and Dougherty, 1996; Wang and Zheng,
Wang and Zheng [1998a] also demonstrated that GA and SA can obtain solutions as good as or better than other traditional optimization methods, and SA outperforms GA in terms of the number of forward simulations required.

To improve the solution efficiency, Skaggs et al. [2001] proposed an enhanced annealing method, which enhanced SA by including “directional search” and “memory” mechanisms and applied the method successfully to a groundwater remediation problem.

SA methods work well on optimization of remediation strategies in discrete or combinatorial forms. However, in combinatorial optimization, each decision variable is restricted to a limited set of possible discrete values, even for variables with continuous values [Dougherty and Marryott, 1991]. This restriction may limit the search for a “true” global optimal solution. SA methods are also very time-consuming due to the large number of forward simulations of groundwater flow and contaminant transport.

2.3.2.3 Tabu Search

The modern form of tabu search (TS) was originally developed by Glover [1986] in an analogy to the human memory process, and a comprehensive introduction of the basic concepts is given by Glover and Laguna [1993]. Similar to SA, TS is based on neighborhood search method with local-optima avoidance. But this is done in a deterministic rather than stochastic way. The central idea of TS is the creation of a “tabu list” to record the previously-seen solutions. The solutions in the tabu list are forbidden in a predefined number of iterations to avoid cycling and to promote a diversified search of the solutions [Reeves, 1996].

Compared with other heuristic methods, the application of TS to the optimization of groundwater remediation design is relatively new. Zheng and Wang [1999b] proposed
a new approach to the problem of simultaneous optimization of well locations and pumping rates. In their application, TS is used to find the optimal well locations, which are discrete decision variables.

In TS method, the length of the tabu list is of great importance since a short list may not be able to prevent the search from previously visited solutions while a long list can cause computational inefficiency [Zheng and Wang, 1999b]. Therefore, in a TS application, the length of the tabu list should be carefully selected. Similar to other heuristic methods, the major computational burden in a TS optimization procedure comes from the forward simulations.

2.3.2.4 Derandomized Evolution Strategy

Similar to GA, derandomized evolution strategy (DES) is also one kind of evolutionary algorithm (EA), a stochastic search technique based on the process of natural evolution [Yoon and Shoemaker, 1999]. DES was first developed by Ostermeier et al. [1994].

Different from the binary strings (chromosomes) used in GA, DES encodes decision variables using real values. In each generation, the new individuals are created by mutations of single parents. The new individuals are then evaluated by calculating the objective function values. Individuals with optimal objective function values will go to the next generation. The procedure is repeated till the stopping criterion is met [Bayer and Finkel, 2004].

Application of DES to optimization of groundwater remediation strategy was introduced by Yoon and Shoemaker [1999] for a time-varying bioremediation case. They showed that DES works better than SGA because DES is more efficient in producing
accurate solutions. *Bayer and Finkel* [2004] further compared the applications of SGA and DES. Their research demonstrates that DES is superior, especially for the case with a large number of wells, and is more robust for the selected advective control problem in their study.

### 2.3.3 Hybrid Methods

As introduced above, for groundwater quality management problems, various optimization methods have been applied. With their own advantages and disadvantages of each method, a common issue for all the methods is the heavy computational burden coming along with the flow and transport simulations. That is because groundwater flow and contaminant transport problems are typically nonlinear. To obtain system responses to specified strategies, the problems need to be solved numerically by either finite difference method (FDM) or finite element method (FEM), which is computationally expensive. To alleviate the computational demands, various optimization methods have been combined and applied together. Sometimes, different optimization techniques are hybridized to take the advantages of both, too.

Among all the combinations, the most commonly used technique is the artificial neural network (ANN). ANN is not actually regarded as an optimization method itself, but often applied together with other optimization methods to alleviate the computational burden from flow and transport simulations. ANN was developed by analogy to the collective processing behavior of neuron in the human brain. They can be trained to derive relationships from examples and from simple linear ones to nonlinear ones that may be very difficult to state explicitly [*Rogers and Dowla*, 1994].
When applied together with other optimization methods, typically ANN is first trained to predict the outcomes of the flow and transport simulations, and is then used to provide system responses to specified remediation strategies. Instead of the high computational demand for numerical simulations, a trained ANN can provide a large number of system responses in a very short time. By taking the place of flow and transport simulations, the efficiency of optimization can be improved significantly. ANN has been applied together with GA [Aly and Peralta, 1999; Johnson and Rogers, 1995; Rogers and Dowla, 1994; Rogers et al., 1995; Yan and Minsker, 2006], and SA [Johnson and Rogers, 2000; Rao et al., 2003].

Although ANN has been applied successfully to approximate the flow and transport simulation, one of the major disadvantages is that hundreds or even thousands of simulation runs are still required to provide data (knowledge base) for training of ANN. If major changes happen to the optimization problem, the knowledge base may need to be recreated. Another disadvantage is that the prior-trained ANN may lead to suboptimal solutions [Yan and Minsker, 2006]. To circumvent this issue, Yan and Minsker [2006] proposed a new dynamic modeling approach called Adaptive Neural Network Genetic Algorithm (ANGA), in which the ANN is trained adaptively and automatically directly within a GA. According to their results, ANGA can save 85 - 90% of the numerical simulations with no loss in accuracy of the optimal solutions.

Johnson and Rogers [2000] compared the uses of ANN and linear approximator (LA) to replace the numerical simulations of flow and transport models in SA optimization methods. They showed that ANN serves better than LA. Morshed and

Response function has also been used to mitigate the computational demand by taking the place of flow and transport simulations. In the work by Zheng and Wang [2002], a simple quadratic response function is used to approximate the system costs and is applied to GA optimization to improve the computational efficiency. However, to generate the response function, simulation models still need to be run numerous times. Moreover, the response function approach is based on the principles of superposition. Therefore, it is only applicable to linear or approximately linear systems.

Zheng and Wang [1999b] proposed a combinational use of TS and LP to optimize well locations and pumping rates simultaneously. Their approach takes advantages of the ability of TS to optimize discrete well location variables and that fact that LP is generally more efficient for optimization of continuous pumping rate variables. In their approach, the complex optimization problem is decomposed into smaller sub-problems to reduce the search space. Application of the linear forward solution-updating procedure [Wang and Zheng, 1998b] improves the computational efficiency further.

The combinational use of GA and DDP has been reported by Chu et al. [2005]. In their approach, GA is used to locate the optimal well locations while DDP is used to decide the optimal pumping rates.

As well as what have been mentioned, the integration of GA and TS techniques can be seen in the work of Kalwij and Peralta [2006], too.
2.4 S/O Application under Uncertainty

When S/O approach is applied to a groundwater quality management problem, the optimization process relies on the numerical simulations to provide responses to various management strategies. In the early optimal designs of the groundwater remediation schemes, the groundwater system is considered to be deterministic. In other words, all the hydrogeologic characteristics regarding the flow and transport simulation at the target site are assumed to be known exactly. Unfortunately, due to the heterogeneous nature of the aquifers, for real-world problems this can never be the case and the groundwater system never lacks uncertainty or uncertain parameters. Uncertainties associated with the simulation results typically come from two sources: the numerical simulation model and the input parameters used in the simulation. Here in this study we assume that the simulation models are accurate and precise, and we only discuss the uncertainties caused by the input parameters.

Uncertainties associated with the groundwater quality management problems is one of the major impediments to effective design of remediation strategies. A direct consequence of the optimization under uncertainty is that the optimal solution obtained may not be optimal, sometimes may not even be feasible, for the real system. Probabilistically, under the situation that the mean values of all the input parameters are assumed to be the “true” values and applied to the optimal remediation design, there is a chance of 50% that the constraints will be violated if the optimal strategy is applied. To account for uncertainty and ensure a certain level of reliability, an “overdesign” may be required. The cost of the overdesign generally increases with the level of model uncertainty and with the desired reliability level [Aksoy and Culver, 2000, 2004; Wagner,
Higher computational source requirement has been another issue when the groundwater system is modeled stochastically to quantify the effects of uncertainty in transport parameters and contaminant distributions.

Therefore, stochastic optimization of remediation strategies under uncertainties has become a very interesting and important research topic. When compared to a deterministic one, a stochastic optimization considers some or all of the system input parameters as stochastic or uncertain. Consequently, system state variables are uncertain as well [Bakr et al., 2003].

In the literature, four major types of formulations exist to accommodate the uncertainties in optimal remediation designs. They are chance-constrained approach, geostatistical approach, feedback control approach, and fuzzy sets approach. In this section, S/O applications on groundwater quality management problems under uncertainty are reviewed by following these four major categories.

### 2.4.1 Chance-Constrained Approach

Chance-constrained approaches have been applied to optimal remediation problems with uncertainties [Sawyer and Lin, 1998; Tiedeman and Gorelick, 1993; Wagner and Gorelick, 1987]. It was developed based on the concept that a stochastic constraint can be expressed deterministically if the state variable is a function of the uncertain parameters [Gorelick, 1997]. In a chance-constrained optimization, the design reliability is incorporated as deterministic chance constraints in the optimization problem based on a probability distribution so that the resulting optimal solution can satisfy the desired reliability [Kalwij and Peralta, 2006].
Wagner and Gorelick [1987] developed a nonlinear chance-constrained model to find optimal aquifer cleanup strategy that satisfies specified water quality standards with a certain reliability. In their formulation, the design reliability is incorporated into the chance constraints. Each chance constraint consists of two parts: the expected value of the state variable and a stochastic component that is used to reflect the specified reliability requirement. The formulation can then be solved deterministically by using nonlinear programming technique. To obtain the statistical information required in the chance constraints, Tiedeman and Gorelick [1993] used the first-order Taylor series approximation, by which the mean and covariance of head could be obtained by using the mean and covariance of aquifer parameters only.

Sawyer and Lin [1998] extended the application of chance-constrained approach to incorporate uncertainties associated with the cost coefficients and constraints of the groundwater management model. They pointed out that a formulation with all coefficients considered uncertain is very useful since uncertainty associated with any of the coefficients exerts an effect on the optimal design.

The chance-constrained approach has also been applied together with feedback control approach, which will be explained in a later section, to find optimal remediation strategy that minimizes the expected remediation cost while satisfying reliability requirement [Lee and Kitanidis, 1991].

The limitation of the chance-constrained approach is apparent: to formulate the reliability into a deterministic chance constraint, the probability distributions of the uncertain parameters are assumed to be known exactly, which can hardly be the case for a real-world problem.
2.4.2 Geostatistical Approach

Geostatistical approach was developed based on multiple equally likely realizations [Gorelick, 1997]. A realization is a set of uncertain parameters generated from the probabilistic model of the uncertain parameters using geostatistical techniques. The basic idea is to find robust solutions that satisfy the constraints for multiple realizations of the uncertain model parameters. This approach has been widely applied to groundwater quality management problems with uncertainties [Aly and Peralta, 1999; Bau and Mayer, 2006; Chan, 1994; Hilton and Culver, 2005; Mantoglou and Kourakos, 2007; Mylopoulos et al., 1999; Smalley et al., 2000; Wagner and Gorelick, 1989; Wagner et al., 1992].

Wagner and Gorelick [1989] used a “stacking” method to provide robust remediation design. This method generates multiple realizations of hydraulic conductivity values in an aquifer and develops a constraint set for each realization. By solving the optimization formulation, a robust optimal design, which satisfies all the constraints simultaneously, can be obtained.

The “stacking” method proposed by Wagner and Gorelick [1987] requires the solution to satisfy all constraints simultaneously without being able to pre-specify the desired system reliability. Chan [1994] proposed a partial infeasible method to allow a specified percentage of the realization to be infeasible to reflect the design reliability. Similar approach was also adopted by Morgan et al. [1993]. Another study of Chan [1993] indicated that the design reliability could be expressed by $N/(N+1)$, where $N$ stands for the number of realizations.
Aly and Peralta [1999] applied GA and ANN to an optimal pump-and-treat design considering the stochastic nature of hydraulic conductivity. In their development, under a specified treatment facility size, the pumping rates are optimized to produce minimum $\text{CMAX}_{(NR)}$, which is the $L_\infty$ norm of contaminant concentrations resulting from a single pumping scheme applied to NR realizations. The optimal solution is then evaluated using Monte Carlo simulation (MCS) to determine its reliability.

In the work of Smalley et al. [2000], a noisy GA was used to obtain optimal remediation design with minimum total costs considering the existence of uncertain hydraulic conductivity. Different from simple GA, in noisy GA the fitness of a string contains a “noise” term, which in their case is the penalty associated with constraints violations. In their formulation, at each generation, the fitness of each string is evaluated by using multiple realizations to allow the consideration of design reliability.

Remediation design using geostatistical approach can be computationally intensive because of the flow and transport simulations associated with each realization. To mitigate the computational burden, Bau and Mayer [2006] used surrogate functions to replace objective functions, which improved computational efficiency significantly. Hilton and Culver [2005] proposed robust GA approach, in which hydraulic conductivity realization varies generation by generation, but only one realization is used for each generation. Ranjithan et al. [1993] demonstrated that out of the large number of realization used in the geostatistical approach, only a few are critical to the optimal design. Therefore, in their work they proposed the use of ANN’s pattern classification ability to find the critical ones from numerous realizations. Their study shows that optimal design based on the critical realizations only is still highly reliable. The critical
realization concept was adopted in a formulation presented by Mantoglou and Kourakos [2007] to achieve computational efficiency.

Another limitation associated with the geostatistical approach is that the obtained solution may be controlled by critical realizations that results in high remediation costs. Since the probability of occurrence of a critical realization can be very low, the approach may end up with a very conservative solution which is very costly [Bakr et al., 2003].

2.4.3 Feedback Control Approach

As it is known, uncertainty associated with aquifer parameters can be reduced during the remediation process if the data collected in the early stages are used to update these parameters [Gorelick, 1997]. Therefore, feedback control has been applied to obtain more reliable remediation strategies [Andricevic and Kitanidis, 1990]. In this technique the differences between predicted variable values via optimization and the measured values are used to guide the modification of the optimal strategy. The process is continued till the end of the remediation process [Aly and Peralta, 1999; Lee and Kitanidis, 1991].

Andricevic and Kitanidis [1990] applied the dual control concept to account for the parameter uncertainties in a pump-and-treat design. The objective function of their formulation is to minimize the expected value of the cost function over the whole remediation horizon. In their formulation, the operation horizon is divided into several management stages. The pumping rates at any stage are optimized based on measurement from previous stages. The pumping rates are optimized with the consideration of both estimation as well as optimization, where estimation is used to reduce the future
predictive uncertainty, while optimization means to improve the decontamination effort. The final solution is decided after weighing both the objectives.

*Lee and Kitanidis* [1991] proposed another formulation named deterministic feedback control. Similar to the work of *Andricevic and Kitanidis* [1990], the dual control concept is applied. The optimal remediation policy is expressed as the sum of a deterministic and a stochastic control term. The former is obtained by solving a deterministic optimization problem, and the latter is calculated by a perturbation approximation to the stochastic optimal control problem. The difference between these two formulations is that in the formulation of *Lee and Kitanidis* [1991], the design reliability is incorporated by using chance-constrained method. Therefore, the obtained optimal design can satisfy the reliability requirement and other constraints.

Weighted feedback law has been applied by *Whiffen and Shoemaker* [1993] to find optimal time-varying pumping rates under parameter uncertainty. The feedback law modifies the pumping scheme for each time period based on the measurements of heads and solute concentrations without requiring specification of which parameters are uncertain. Different from the dual control, feedback laws don’t update or improve the parameter values but change the pumping policy directly according to the observed differences in heads and concentrations. With its advantages though, this method can be only applied to DDP formulations since other optimization techniques such as NLP does not generate any form of a feedback law.

### 2.4.4 Fuzzy Sets Approach

Other than probability theory, fuzzy sets theory has also been applied to describe uncertainty in single or multiple aquifer parameters for groundwater quality management.
problems with uncertainties [Guan and Aral, 2004, 2005]. Fuzzy sets theory was developed by Zadeh [1965] to handle uncertain or vague information. According to fuzzy sets theory, the degree that an element belongs to a fuzzy set is called the degree of membership, which can be evaluated from the membership function.

Guan and Aral [2004] proposed an application of fuzzy sets theory to optimal pump-and-treat remediation design under uncertain hydraulic conductivities. In the two proposed optimization models, the hydraulic conductivity uncertainties were described using fuzzy sets, while the pumping schedules were described as crisp and fuzzy, respectively. The models were then transformed into computational models using fuzzy set theory, which were then solve using optimization algorithms such as golden section search method, genetic algorithm, and direct comparison method. The numerical results indicated that the optimization formulations using fuzzy sets theory were flexible and reliable.

A limitation associated with the above models is the computational cost, especially for large-scale problems. Therefore, a genetic algorithm embedded with fuzzy vertex algebra was developed by Guan and Aral [2005] to improve the computational efficiency, which was demonstrated to be the case. In their work, the previous models were also expanded to fit large scale applications with multiple pumping wells multiple uncertain parameters, such as hydraulic conductivity and longitudinal and transverse dispersion coefficient, where were interpreted using fuzzy sets.

2.5 Sensitivity Analysis and Uncertainty Analysis

A physical system can be characterized by independent variables, dependent variables, and relationships between these quantities. The relationships can sometimes be
simulated using numerical simulation models. For example, the groundwater flow in a subsurface system can be simulated using simulation model MODFLOW, in which the independent variables include hydraulic conductivities, recharge rate, extraction rates in pumping wells, and etc., the dependent variables are head values in the groundwater system, and the relationship between them can be interpreted by using governing equation (2.3).

Owing to the incomplete knowledge or uncertainty regarding the independent variables (input parameters) and numerically methods applied to the simulation models, there are always uncertainties associated with the dependent variables (simulation results). It is well known that it is extremely hard, if not impossible, to model a real-world groundwater system precisely due to the heterogeneities of the hydraulic aquifer properties, and the heterogeneities can strongly influence the behavior of such systems.

To quantify the uncertainties in the results, sensitivity and uncertainty analyses are considered as formal methods. In general, a sensitivity analysis is used to quantify the effects of input variations on the simulation results, meanwhile an uncertainty analysis is used to assess the effects of input uncertainties on the uncertainties in computed results [Ionescu-Bujor and Cacuci, 2004].

2.5.1 Sensitivity Analysis

Sensitivity analysis has been applied to identify critical control points, screen important input parameters, and validate simulation models [Frey and Patil, 2002]. In sense of scope, sensitivity analyses can be either local or global. The objective of a local sensitivity analysis is to analyze the system response around a chosen point, while the
objective of a global sensitivity analysis is to find all the critical points for the system [Ionescu-Bujor and Cacuci, 2004].

In this part of the review, only some of the most popular sensitivity analysis methods that have been applied to groundwater problems are introduced. Other than those, more information can be found in works of Frey and Patil [2002] and Ionescu-Bujor and Cacuci [2004], which give extensive reviews of sensitivity analysis methods applied to various engineering disciplines.

2.5.1.1 Brute-Force Method

Brute-Force method, which is also called finite difference perturbation method, is the simplest way of calculating local sensitivities. Assuming there is a simulation model of the form

$$C = f(u),$$  \hfill (2.5)

where $C$ is the target value, which is a function of $u$, and $u$ is a input parameter vector with $I$ entries $u_1, u_2, ..., u_I$. The sensitivities at a chosen point $u^0$ are estimated by using a finite difference perturbation:

$$\left( \frac{\partial C}{\partial u_i} \right)_{u^0} = \frac{f(u^0, ..., u_i^0 + \delta u_i, ..., u_I^0) - f(u^0)}{\delta u_i} \text{ for } (i = 1, ..., I).$$ \hfill (2.6)

If a forward- or backward-difference method is applied, $(I+1)$ evaluations of $C$ values are required to obtained sensitivities of $C$ with respect to all the input parameters. Otherwise, if a central-difference is desired, number of $C$ value evaluations needs to be increased to $2I$. 

46
Brute-Force method is conceptually straightforward but computationally expensive. And the increment value $\delta u_i$ should be chosen carefully to avoid erroneous sensitivity results [Ionescu-Bujor and Cacuci, 2004].

### 2.5.1.2 Adjoint Sensitivity Analysis Procedure

Adjoint sensitivity analysis procedure (ASAP) is a deterministic sensitivity analysis method which is typically more accurate and computationally efficient than the Brute-Force method [Bakr and Butler, 2005]. It has been applied by Bakr et al. [2003] and Bakr and Butler [2005] to calculate sensitivity coefficients for various uncertainty analyses.

To illustrate the basic concepts used in ASAP as stated in the work of Bakr et al. [2003], assume that there exists a simulation model

$$g(s,u) = 0,$$

where $s$ is the state variables vector, and $u$ is the input parameters vector.

Considering there is a vector of performance criteria $j(s,u)$, which are functions of $s$ and $u$. The sensitivity of performance criteria $j$ with respect to input parameters $u$ can be expressed as

$$\frac{dj}{du} = \frac{\partial j}{\partial u} + \frac{\partial j}{\partial s} \frac{s}{u}.$$  

Differentiating equation (2.7) with respect to $u$ leads to

$$\frac{\partial g}{\partial u} + \frac{\partial g}{\partial s} \frac{s}{u} = 0,$$  

and

$$\frac{s}{u} = -\left[ \frac{\partial g}{\partial s} \right]^{-1} \frac{\partial g}{\partial u}.$$  

Substituting (2.10) into (2.8) yields

\[ \frac{dj}{du} = \frac{\partial j}{\partial u} - \frac{\partial j}{\partial s} \left[ \frac{\partial g}{\partial s} \right]^{-1} \frac{\partial g}{\partial u} . \]  \hspace{1cm} (2.11)

By defining a matrix of adjoint variables \( A \) as

\[ \left[ \frac{\partial g}{\partial s} \right]^T \ A = - \left[ \frac{\partial j}{\partial s} \right]^T , \]  \hspace{1cm} (2.12)

it can be obtained that

\[ A^T = - \frac{\partial j}{\partial s} \left[ \frac{\partial g}{\partial s} \right]^{-1} . \]  \hspace{1cm} (2.13)

Therefore (2.11) can be written as

\[ \frac{dj}{du} = \frac{\partial j}{\partial u} + A^T \frac{\partial g}{\partial u} . \]  \hspace{1cm} (2.14)

The sensitivity of performance criteria \( j \) with respect to input parameters \( u \) can be calculated either by solving (2.10) and substituting the results to (2.8) or by solving (2.13) and substituting the adjoint matrix \( A \) into (2.14). The former method is called forward sensitivity analysis procedure (FSAP) and the latter is called adjoint sensitivity analysis procedure (ASAP). From the description, it can be seen that when the number of input parameters is larger than the number of state variables, which is the case for most large-scale flow and transport problems, ASAP is computationally more efficient.

2.5.2 Uncertainty Analysis

According to different causes, uncertainties can be put into two categories – stochastic uncertainty and subjective uncertainty. Stochastic uncertainty, which is also called intrinsic uncertainty, is a property of the studied system itself since it’s caused by various behavior patterns of the system, while subjective uncertainty (information
uncertainty), which is caused by the inability to provide the exact input data, is a property of the analysis [Helton and Davis, 2002; Ionescu-Bujor and Cacuci, 2004]. Stochastic uncertainty is not of the interest of this study and therefore only uncertainty analysis methods regarding the subjective uncertainty are discussed here.

The most basic uncertainty analysis method is analytical uncertainty analysis methods, in which the probability density function and/or statistical moments can be derived analytically based on the statistical properties of the input parameters and the relationships between the input and output parameters. Unfortunately, the application of the analytic methods toward a real-world problem is prohibitive because of its requirements such as simple functional relationships and independence of stochastic variables [Tung and Yen, 2005]. Generally, two groups of methods have been widely applied to assess the uncertainties associated with the groundwater flow and contaminant fate and transport models – the Monte Carlo simulation (MCS) methods and the first and second moment methods.

2.5.2.1 Monte Carlo Simulation Method

Monte Carlo simulation (MCS) is a statistical uncertainty analysis method, which evaluates the distribution of system responses subject to input uncertainties by measuring system responses repeatedly under various realizations of input generated according to their probabilistic distributions [Tung and Yen, 2005].

In an MCS application, given the probability distributions of the input variables, numerous equal-likely realizations are generated. Simulations are conducted repeatedly by using these realizations as input. The simulation results are then collected and
analyzed statistically to provide the probability distribution and statistical properties of the output variables of interest.

MCS is conceptually straightforward and can be easily applied without even knowing details about the simulation models. Therefore, it has been considered to be the main tool to be used in groundwater hydrology in assessing the uncertainties in groundwater flow and contaminant transport predictions caused by input uncertainties [Ballio and Guadagnini, 2004]. Application of MCS can be seen in works of James and Oldenburg [1997], Hassan et al. [1998b], Naff et al. [1998a; Naff et al., 1998b], Salandin and Fiorotto [1998], and van Leeuwen et al. [1998], just to name a few. MCS has also been applied often to provide results for verification purposes [e.g., Bakr and Butler, 2005; Chin and Wang, 1992; Ferrante and Yeh, 1999; Foussereau et al., 2000; Hassan et al., 1998a].

Although the MCS approach has been widely applied, it has several disadvantages. One major disadvantage is the large number of simulation runs [Andricevic, 1993]. The accuracy of the stochastic properties obtained from the MCS is a function of the number of simulation runs. Especially, for models with numerous uncertain variables and for which low probabilities (< 0.1) are of interest, a large amount of simulations may be required [Tung and Yen, 2005]. Another disadvantage is that, as it is well known, there is not well-established convergence criterion for Monte Carlo simulations [Ballio and Guadagnini, 2004]. Therefore, a given number of more simulations runs may be required to check the convergence.
2.5.2.2 First and Second Moment Method

The first and second moment methods are deterministic uncertainty analysis methods that have been widely used in groundwater studies. The basic assumption for these methods is that the uncertainty regarding the variables of interest can be summarized with the mean (the first moment) and the variance-covariance (the second moment) [Dettinger and Wilson, 1981].

The first and second moment methods can be applied in two major ways: perturbation and Taylor series expansion. The perturbation method works by perturbing the partial differential governing equation slightly to obtaining a new equation that governs the random component of the target variables [Dettinger and Wilson, 1981]. Numerous works exist in literature regarding the use of perturbation methods for derivation of stochastic moments of piezometric head and solute concentration in groundwater systems [e.g., Bakr et al., 1978; Gutjahr et al., 1978; Sagar, 1978]. However, most of these applications concentrate on intrinsic uncertainty analysis.

Compared with perturbation methods, Taylor series expansion methods are more often applied to the evaluation of subjective uncertainties, which are caused by incomplete input information [e.g., Bakr et al., 2003; Bakr and Butler, 2005; Ferrante and Yeh, 1999; Tiedeman and Gorelick, 1993; Wagner and Gorelick, 1987]. Dettinger and Wilson [1981] gave a detailed introduction to the first- and second-order Taylor series expansion analysis method. Derivation of the first-order approximation method, as explained in the work of Ionescu-Bujor and Cacuci [2004], is described as follows.

Assuming that there is a model of the form

\[ C = f (u_1, \ldots, u_I) = f (u_1^0 + \delta u_1, \ldots, u_I^0 + \delta u_I). \]  \hspace{1cm} (2.15)
Parameters \((u_1, \ldots, u_I)\) are random variables with a joint probability density function \(p(u_1, \ldots, u_I)\) and means, variances, covariances as follows, respectively:

\[
E(u_i) = u_i^0; \quad \text{(2.16)}
\]

\[
\text{var}(u_i, u_j) \equiv \sigma_i^2 \equiv \int_{S_u} (u_i - u_i^0)^2 p(u_1, \ldots, u_I) \, du_1 \ldots du_I; \quad \text{(2.17)}
\]

\[
\text{cov}(u_i, u_j) \equiv \int_{S_u} (u_i - u_i^0)(u_j - u_j^0) p(u_1, \ldots, u_I) \, du_1 \ldots du_I. \quad \text{(2.18)}
\]

According to Taylor series, the expansion of \(f\) around the nominal values \(u^0 = (u_1^0, \ldots, u_I^0)\) up to the \(n\)th order can be written as

\[
f(u_1, \ldots, u_I) \equiv f(u_1^0 + \delta u_1, \ldots, u_I^0 + \delta u_I)
= f(u^0) + \sum_{i=1}^I \left( \frac{\partial f}{\partial u_i} \right)_{u^0} \delta u_i
+ \frac{1}{2} \sum_{i=1}^I \sum_{j=1}^I \left( \frac{\partial^2 f}{\partial u_i \partial u_j} \right)_{u^0} \delta u_i \delta u_j
+ \frac{1}{3!} \sum_{i=1}^I \sum_{j=1}^I \sum_{k=1}^I \left( \frac{\partial^3 f}{\partial u_i \partial u_j \partial u_k} \right)_{u^0} \delta u_i \delta u_j \delta u_k + \ldots.
\quad \text{(2.19)}
\]

The first-order approximation of \(f\) can be written as

\[
f(u_1, \ldots, u_I) = f(u^0) + \sum_{i=1}^I \left( \frac{\partial f}{\partial u_i} \right)_{u^0} \delta u_i
= C^0 + \sum_{i=1}^I S_i \delta u_i, \quad \text{(2.20)}
\]

where

\[
C^0 \equiv f(u^0), \quad \text{(2.21)}
\]

and the sensitivity of \(C\) to the parameter \(u_i\)

\[
S_i \equiv \left( \frac{\partial f}{\partial u_i} \right)_{u^0}.
\quad \text{(2.22)}
\]

According to (2.20), the mean value of \(C\) can be obtained as

\[
E[C] \equiv C^0 + \int_{S_u} \left( \sum_{i=1}^I S_i \delta u_i \right) p(u_1, \ldots, u_I) \, du_1 \ldots du_I = C^0. \quad \text{(2.23)}
\]
The \( l \)th moment of \( C \) can be calculated by (2.20) and (2.23):

\[
\mu_l(C) \equiv E[(C - E[C])^l] = \int_{u_i} \left( \sum_{i=1}^{I} S_i \delta u_i \right)^l p(u_1, \ldots, u_l) du_1 \ldots du_l .
\]  

(2.24)

Especially, the variance of \( C \), which is the second moment, can be expressed as

\[
\text{var}(C) = \int_{u_i} \left( \sum_{i=1}^{I} S_i \delta u_i \right)^2 p(u_1, \ldots, u_l) du_1 \ldots du_l = SV_\delta S^T ,
\]

(2.25)

where \( S \) is the sensitivity vector

\[
S = \left[ \left( \frac{\partial C}{\partial u_1} \right)_{u_0}, \ldots, \left( \frac{\partial C}{\partial u_I} \right)_{u_0} \right]^T ,
\]

(2.26)

and \( V_\delta \) denotes the covariance matrix with elements defined as

\[
(V_\delta)_{ij} = \begin{cases} \text{cov}(u_i, u_j) = \rho_{ij} \sigma_i \sigma_j & (i \neq j, \rho_{ij} = \text{correlation coefficient}) \\ \text{var}(u_i) = \sigma_i^2 & (i = j) \end{cases} .
\]

(2.27)

Derivation of higher-order analysis method is similar, and therefore is not given here. For the applications of Taylor series expansion methods to real-world problems, although higher-order approximation has been tested and applied [Dagan, 1985], typically the first-order approximation is used. Dagan [1985] indicated in his work that for the case of head variances in steady aquifer flow, the first-order approximation is very robust, and the second-order correction is smaller than 10% of the first-order approximation. When the first and second moments of output variables are calculated by using first-order approximation, this method is often called first-order second moment (FOSM) method.

The Taylor series expansion methods have been widely applied to assess the uncertainties for various kinds of groundwater problems. For example, Bakr and Butler [2005] applied a first-order approximation to evaluate the uncertainty associated with the well capture zone. In the work of Wagner and Gorelick [1987], first-order approximation
was used to evaluate the mean and variance of contaminant concentration so that a stochastic constraint for a groundwater quality management problem can be turned into a deterministic one.

The Taylor series expansion methods have their own limitations, too. One limitation is that they will work well only for nonlinear systems with “reasonably small” coefficients of variation [Dettinger and Wilson, 1981]. Another drawback for these methods is that, when applied to a complex and nonanalytical real-world problem, computations of sensitivity coefficients have to be done numerically and can be very time consuming [Tung and Yen, 2005].

2.6 Summary

In this chapter, the applications of S/O to groundwater quality management problems are reviewed. Optimal remediation design by using S/O has been widely studied because of the high costs associated with groundwater remediation systems and the ability of S/O to find the most cost-efficient remediation strategy. In an S/O approach, the simulation models are used to predict the system responses with respect to specified remediation strategies, while the optimization techniques are used to find the optimal one.

An optimal remediation design problem using S/O approach typically consists of four parts: flow and transport simulators, formulation of the optimization problem, incorporation of the simulators into the formulation, and optimization techniques. All the flow and transport simulators are based on governing equations (2.1) and (2.2). The major difference between various simulators is the numerical solution technique, which can be either FDM or FEM.
Various optimization techniques have been applied to obtain the optimal remediation design complying different management objectives and constraints. In the optimization of groundwater remediation strategy using S/O approach, most of the computational demand attributes to the numerical simulations of flow and transport model regardless of the optimization techniques. This is because in an S/O approach the simulators need to be run repeatedly to provide system responses to various policies. Especially, for a complex field-scale system, simulation of flow and transport regarding to one specific strategy may take hours of CPU time. The heavy computational burden has hindered the application of S/O approach to real-world problems. At the end of this chapter, sensitivity and uncertainty analyses that have been applied to various groundwater problems are also reviewed.
CHAPTER 3

SENSITIVITY ANALYSIS OF CAMP LEJEUNE MODEL

Groundwater contamination may cause serious health issues when human beings are exposed to the contaminants in the groundwater through all kinds of daily activities. Environmental epidemiologic studies are designed to reveal relationships between exposures to these contaminants and the health effects. However, epidemiologic studies are often retrospective and there is only limited quantitative historical information available to conduct an exposure assessment. To provide exposure data for the epidemiologic studies, historical reconstruction and simulation analyses are frequently used [Maslia et al., 2003; Nieuwenhuijzen et al., 2006].

ATSDR is conducting an epidemiologic study to evaluate whether exposures (in-utero and during infancy – up to 1 year of age) to volatile organic compounds (VOCs) existing in the contaminated drinking water at the U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers that were observed at the site. The study includes the births that occurred to women who were pregnant while they resided in the family housing at the base during the period 1968 – 1985. There is no exposure data and very limited site-specific contamination data are available to support the epidemiologic study. As a result, ATSDR is using modeling techniques to estimate the historical and present-day contamination conditions in the groundwater and the water treatment plant (WTP) at Camp Lejeune, North Carolina [Maslia et al., 2007a].
During the historical reconstruction study, PCE (Tetrachloroethylene) and its degradation by-products were found to be the major contaminants. The groundwater flow and fate-and-transport of contaminants in Tarawa Terrace area of the Camp Lejeune base and its vicinity have been simulated to evaluate the contaminant concentrations at the WTP. Due to the nature of the historical reconstruction, there is inevitably uncertainty residing in the reconstructed input data, and therefore the final results, of these simulations, which may significantly impact the reliability of the related epidemiologic study.

This study is to evaluate the uncertainties residing in the simulation results of the Camp Lejeune model by ATSDR, which include PCE concentrations and PCE MCL arrival time at the Tarawa Terrace WTP. Considering that a large number of input variables are applied in the simulation models, sensitivity analyses are necessary to screen out the most critical uncertain variables prior to the uncertainty analysis. Uncertainty analysis using only the critical uncertain variables can yield highly reliable results, while the computational demand associated with the analysis can be significantly reduced.

3.1 Introduction to Camp Lejeune Model

3.1.1 Historical Background

U.S. Marine Corps Base Camp Lejeune is located near Jacksonville, Onslow County, North Carolina. The Agency for Toxic Substances and Disease Registry (ATSDR), U.S. Department of Health and Human Services, is conducting an epidemiologic study at this site to determine if exposure to contaminated drinking water

Due to limited exposure data available for the period of interest (POI, 1968 – 1985), ATSDR has undertaken a reconstruction of the historical data. The investigation focuses on the Tarawa Terrace area and its vicinity (Figure 3.1). The Tarawa Terrace area is bounded on the east by Northeast Creek, and to the south by New River and Northeast Creek. On the west and north, it is bounded by the drainage boundaries of these streams. The historical reconstruction includes the groundwater system reconstruction, contaminant source characterization, and contaminant fate-and-transport simulation in the groundwater system and the water distribution system (WDS) serving the Tarawa Terrace area.

Figure 3.1. Water-supply well locations at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina. (from Maslia et al. [2007b])
The study by ATSDR concluded that groundwater was the sole source of water to the WTP and the WDS serving the Tarawa Terrace area. The source of contaminants in the groundwater was the ABC One-Hour Cleaners located to the north of several water-supply wells at Tarawa Terrace (Figure 3.1). According to the study, Tetrachloroethylene (PCE) was the major contaminant, and was continuously released to the subsurface system at a rate of 1,200 gram/day during the period of January 1953 to December 1984. PCE released from ABC One-Hour Cleaners migrated into the groundwater system and was then transported into the WTP by the water-supply wells shown in Figure 3.1.

Based on the study of the hydrogeologic and historical data regarding the Tarawa Terrace area and its vicinity, the ATSDR modeling team reconstructed and simulated the multilayer groundwater flow at the site using MODFLOW, a groundwater flow simulation model [McDonald and Harbaugh, 1988]. Simulation model MT3DMS [Zheng and Wang, 1999a] was then used to evaluate the fate-and-transport of PCE in the subsurface. Based on this analysis, the PCE concentration distribution and MCL arrival time at the WTP were determined historically.

In both of the MODFLOW and MT3DMS models, the Tarawa Terrace area and its vicinity are discretized into 200 rows, 270 columns, and 7 layers. The simulated time period spans from January 1951 to December 1994 with each month being considered as one stress period – January 1951 is named “Stress Period 1,” and December 1994 is named “Stress Period 528.”

In the Camp Lejeune model, a total of 16 water-supply wells were used to supply groundwater to the Tarawa Terrace WTP. Thirteen of these wells are located in the Tarawa Terrace area and its vicinity (Figure 3.1). The other three wells, identified as well
6, well 7, and well TT-45, are located outside of this area, and therefore, are assumed to have zero contaminant concentration, which implies that these wells contributed only water but no contaminant mass to the WTP.

In MODFLOW and MT3DMS simulations, the location of a pumping well is identified in terms of the coordinates of the cell in which the well lies – \((x, y, z)\). The \(x\), \(y\), and \(z\) values are corresponding to the layer number, row number, and column number of the cell, respectively. According to the well-construction logs, some wells penetrate more than one layer of aquifer, therefore in MODFLOW simulations some well discharges are split into two or more “virtual” wells which extract water from different layers. For example, in the MODFLOW input used by the ATSDR, well TT-52 is split into TT-52A and TT-52B, where the extension “A” refers to Layer-1 and “B” refers to Layer-3. Wells TT-31 and TT-54 also are split this way. In this study well TT-53 and TT-67 are split to satisfy their pumping capacities, with respect to dry- and wet-cell conditions observed at the cell. During the simulation period (1951 – 1994), the pumping rates of the water-supply wells varied, and some wells were out of service for some stress periods. Locations and service periods of these water-supply wells are listed in Table 3.1. Using the historical records, the pumping rates and pumping capacities of the water-supply wells were generated for all the stress periods.
Table 3.1. Locations and service periods of water-supply wells in Tarawa Terrace area

<table>
<thead>
<tr>
<th>Well</th>
<th>Layer</th>
<th>Row</th>
<th>Column</th>
<th>Start Date</th>
<th>End Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>TT-23</td>
<td>3</td>
<td>84</td>
<td>175</td>
<td>08/1984</td>
<td>04/1985</td>
</tr>
<tr>
<td>TT-25</td>
<td>3</td>
<td>67</td>
<td>194</td>
<td>01/1982</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-26</td>
<td>3</td>
<td>61</td>
<td>184</td>
<td>01/1952</td>
<td>01/1985</td>
</tr>
<tr>
<td>TT-27</td>
<td>3</td>
<td>52</td>
<td>135</td>
<td>01/1952</td>
<td>12/1961</td>
</tr>
<tr>
<td>TT-28</td>
<td>3</td>
<td>47</td>
<td>96</td>
<td>01/1952</td>
<td>12/1971</td>
</tr>
<tr>
<td>TT-29</td>
<td>3</td>
<td>41</td>
<td>61</td>
<td>01/1952</td>
<td>06/1958</td>
</tr>
<tr>
<td>TT-30</td>
<td>3</td>
<td>47</td>
<td>97</td>
<td>01/1972</td>
<td>01/1985</td>
</tr>
<tr>
<td>TT-31A</td>
<td>1</td>
<td>104</td>
<td>152</td>
<td>01/1973</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-31B</td>
<td>3</td>
<td>104</td>
<td>152</td>
<td>01/1973</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-52A</td>
<td>1</td>
<td>101</td>
<td>136</td>
<td>01/1962</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-52B</td>
<td>3</td>
<td>101</td>
<td>136</td>
<td>01/1962</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-53A</td>
<td>1</td>
<td>81</td>
<td>151</td>
<td>01/1962</td>
<td>01/1984</td>
</tr>
<tr>
<td>TT-53B</td>
<td>3</td>
<td>81</td>
<td>151</td>
<td>01/1962</td>
<td>01/1984</td>
</tr>
<tr>
<td>TT-54A</td>
<td>1</td>
<td>106</td>
<td>167</td>
<td>01/1962</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-54B</td>
<td>3</td>
<td>106</td>
<td>167</td>
<td>01/1962</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-55</td>
<td>1</td>
<td>53</td>
<td>136</td>
<td>01/1962</td>
<td>12/1971</td>
</tr>
<tr>
<td>TT-67A</td>
<td>1</td>
<td>93</td>
<td>158</td>
<td>01/1972</td>
<td>02/1987</td>
</tr>
<tr>
<td>TT-67B</td>
<td>3</td>
<td>93</td>
<td>158</td>
<td>01/1972</td>
<td>02/1987</td>
</tr>
</tbody>
</table>

3.1.2 Simulation Results of ATSDR Modeling Study

In the ATSDR study, the PCE concentration at the WTP was evaluated by employing the following steps as indicated in Figure 3.2:

i. MODFLOW model was used to simulate the groundwater flow in the Tarawa Terrace area and its vicinity. The MODFLOW simulation also generated the flow-transport link (FTL) file to be used in the MT3DMS simulation;

ii. Using the FTL file, along with other input files, MT3DMS simulation was conducted to obtain the PCE concentrations in the water-supply wells; and

iii. The PCE concentration distribution obtained from MT3DMS simulation is used to calculate the PCE concentration at the WTP through a volumetric mixing model.
The PCE concentration distribution in the water-supply wells obtained from step (ii) is illustrated in Figure 3.3. To distinguish the pumping schedule used in the ATSDR model from the other updated pumping schedules to be discussed in later chapters, it is identified as the “Original Schedule” (Org. Sche.) in the figure as well as throughout the remainder of this thesis. The PCE concentrations in the water-supply wells are shown during their service periods as listed in Table 3.1. Although 16 pumping wells were operating in the Tarawa Terrace area in ATSDR’s simulation, only wells TT-23, TT-25, TT-26, TT-54A, TT-54B, and TT-67 had PCE concentrations higher than the PCE MCL (5 ppb). Among these wells, well TT-26 had a much longer period of exposure to PCE concentrations over 5 ppb – the PCE MCL arrival time at well TT-26 is January 1957, while the second-earliest PCE MCL arrival in a water-supply well occurred during January 1983 at well TT-54A. PCE concentration at well TT-26 is always much higher than in the other water-supply wells, indicating that TT-26 conveyed the majority of PCE mass introduced into the WTP. This fact might be caused by the proximity of well TT-26 to the contaminant source and its long pumping history.
Employing the PCE concentration data at the water-supply wells, along with the pumping rates in these wells, the PCE concentration in the Tarawa Terrace WTP was calculated by using the following volumetric mixing model:

$$C_i = \frac{\sum_{j=1}^{n} q_{ij} c_{ij}}{Q_{Ti}}$$

(3.1)

in which $C_i$ is the PCE concentration at the WTP at stress period $i$ (ML$^{-3}$); $n$ is the total number of active water-supply wells in stress period $i$; $q_{ij}$ is the pumping rate of well $j$ at stress period $i$ (L$^3$T$^{-1}$); $c_{ij}$ is the PCE concentration in the water-supply well $j$ at stress period $i$ (ML$^{-3}$); and $Q_{Ti}$ is the total water demand at stress period $i$ (L$^3$T$^{-1}$).
The PCE concentration in the Tarawa Terrace WTP obtained from the ATSDR model is shown in Figure 3.4. According to the figure, the PCE concentration at the WTP first exceeded the 5ppb MCL during November 1957. Recall that by this time only well TT-26 had a PCE concentration higher than 0.001 ppb, indicating well TT-26 is the critical well in assessing the PCE MCL arrival time at the WTP.

As illustrated in Figure 3.4, the maximum PCE concentration at the WTP is 183.04 ppb and the minimum one is 0.72 ppb for the period of interest. During this period, however, there are only 15 months during which the PCE concentration at the WTP is lower than 46.69 ppb. Therefore, for most of the POI (201 months out of 216
months), the PCE concentration in the Tarawa Terrace WTP ranges between 46.69 ppb and 183.04 ppb, and the average PCE concentration is about 86.39 ppb, which is much higher than the 5 ppb MCL.

The time periods in which the PCE concentration at the WTP is lower than 46.69 ppb are: July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985. These are also time periods during which well TT-26 was out of service. As can be seen in Figure 3.3, during these time periods, PCE concentrations in other water-supply wells were much less than those at well TT-26. Stopping well TT-26 from supplying water to the WTP, therefore, caused the sudden PCE concentration declines as shown in Figure 3.4.

The reason for the PCE concentration decline at the end of 1961 (Figure 3.4) is similar to the one described previously. At that time, the pumping rate of well TT-26 decreased from 28,715 ft³/day to 18,959 ft³/day, while the total water supplied to the WTP remained unchanged (116,199 ft³/day). Because PCE concentrations at other water-supply wells were negligible (less than 0.001 ppb) and well TT-26 was the only source of PCE to the WTP at that time, a decrease of PCE concentration was expected at the WTP.

3.2 Sensitivity Analyses of Uncertain Variables in Camp Lejeune Model

3.2.1 Uncertain Variables Identification

Three numerical models have been applied in the ATSDR study to obtain the PCE concentration in Tarawa Terrace WTP: MODFLOW, MT3DMS, and the volumetric mixing model. Prior to the sensitivity analyses, study of the input data for these three models identifies the uncertain variables used in these models.
As illustrated in Figure 3.5, uncertain variables applied in the MODFLOW simulation include storage coefficient, hydraulic conductivities, recharge rate, and pumping schedule. Uncertain parameters for the MT3DMS simulation include first order reaction rate, distribution coefficient, mass loading rate, bulk density, longitudinal dispersivity, and effective porosity. For the volumetric mixing model, the uncertain input is pumping schedule. All the uncertain variables explained above take uncertainties into the simulated PCE concentration in Tarawa Terrace WTP, and therefore the PCE MCL arrival time at the WTP.

![Figure 3.5. Uncertain variables applied in Camp Lejeune model](image)

### 3.2.2 Sensitivity Analyses of Uncertain Variables in Camp Lejeune Model

Among all the uncertain variables identified in Figure 3.5, pumping schedule is a very unique one because it takes uncertainties into the final results through two different
pathways – the MODFLOW simulation and the volumetric mixing model. It is also special due to the fact that, as an often utilized property in groundwater management problems, manipulation of pumping schedules can cause dramatic changes in groundwater flow and contaminant fate-and-transport. Therefore, while the sensitivity analyses regarding the remaining uncertain parameters are discusses in this chapter, the changes of PCE concentrations and MCL arrival times at the WTP caused by pumping schedule variations will be evaluated separately in the next chapter.

During the sensitivity analysis process, the uncertain parameters used in the Camp Lejeune model were varied one at a time. The sensitivity of each uncertain variable is evaluated from two aspects: (i) the change of PCE MCL arrival time at the WTP caused by the parameter variation; and (ii) the effect of parameter variation on the change of PCE concentration at the WTP during POI, which is quantified by the relative change, the average of relative change, and the average of absolute relative change of PCE concentration at the WTP.

The relative change of PCE concentration is calculated by

$$RC_{ij} = \frac{C_{ij} - C_{i0}}{C_{i0}} \times 100\%,$$

where $RC_{ij}$ is the relative change of PCE concentration in stress period $i$ of simulation $j$ (%); $C_{ij}$ is the PCE concentration in stress period $i$ of simulation $j$ (ML$^{-3}$); and $C_{i0}$ is the PCE concentration in stress period $i$ of the ATSDR model (ML$^{-3}$). Due to the low PCE concentrations at the WTP, the relative changes of PCE concentrations are significantly large during the stress periods that well TT-26 was out of service (07/1980 – 08/1980, 01/1983 – 02/1983, and 02/1985 – 12/1985). Therefore, PCE concentrations in these stress periods were eliminated from the analysis.
The average of relative change of PCE concentration at the WTP is calculated by

$$
\overline{RC}_j = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{C_{ij} - C_{i0}}{C_{i0}} \right) \times 100\% ,
$$

(3.3)

where $\overline{RC}_j$ is the average of relative change for simulation $j$ (%); and $N$ is the total number of stress periods in one simulation, which is 201 in this case.

The average of absolute values of relative change is calculated by

$$
\overline{|RC|}_j = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{C_{ij} - C_{i0}}{C_{i0}} \right| \times 100\% ,
$$

(3.4)

where $\overline{|RC|}_j$ is the average of absolute relative change for simulation $j$ (%).

During the sensitivity analysis, the three values of each uncertain variable were calculated and compared, based on which the critical uncertain variables were selected. The sensitivity analysis results are discussed parameter by parameter as follows.

3.2.2.1 Storage Coefficient

Storage coefficients are variables applied in the Block-Centered Flow package of the MODFLOW simulation. They consist of primary storage coefficients and secondary coefficients. For simulated unconfined layer, the primary storage coefficient stands for specific yield ($S_y$), while for layer varying between being confined and unconfined (confined/unconfined) it means confined storage coefficient ($S_s$). The secondary coefficient is only applicable for confined/unconfined layer and is always the specific yield of the layer. According to the sensitivity analysis results, changes of the secondary coefficients for layers 2 – 7 cause no change to the final results. Therefore, only specific yield in layer 1 and storage coefficients for layers 2 – 7 are discussed here.
The specific yields in layer 1 have a constant value of 0.5 in the ATSDR model. For sensitivity analysis, the values were varied between 0.1 and 1.0. The analysis results are plotted in Figure 3.6 and summarized in Table 3.2. Figure 3.6 indicates that the variation of the specific yield in layer 1 can cause relative changes of PCE concentration at the WTP from -2.78% to 3.33%. Considering that the specific yield is changed by -80% to +100%, the PCE concentration at the WTP is relatively insensitive to the change of specific yield in layer 1. Results in Table 3.2 also indicate that the variation of specific yield during the analysis causes no change of PCE MCL arrival time at the WTP.

Figure 3.6. Sensitivity analysis results for specific yield in layer 1
Table 3.2. Sensitivity analysis results for specific yield in layer 1

<table>
<thead>
<tr>
<th>Specific Yield in Layer 1</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>83</td>
<td>0</td>
<td>1.54</td>
<td>-2.78</td>
<td>-0.31</td>
</tr>
<tr>
<td>0.02</td>
<td>83</td>
<td>0</td>
<td>1.12</td>
<td>-2.08</td>
<td>-0.24</td>
</tr>
<tr>
<td>0.03</td>
<td>83</td>
<td>0</td>
<td>0.71</td>
<td>-1.38</td>
<td>-0.17</td>
</tr>
<tr>
<td>0.04</td>
<td>83</td>
<td>0</td>
<td>0.34</td>
<td>-0.69</td>
<td>-0.09</td>
</tr>
<tr>
<td>0.05</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.06</td>
<td>83</td>
<td>0</td>
<td>0.67</td>
<td>-0.34</td>
<td>0.08</td>
</tr>
<tr>
<td>0.07</td>
<td>83</td>
<td>0</td>
<td>1.35</td>
<td>-0.65</td>
<td>0.17</td>
</tr>
<tr>
<td>0.08</td>
<td>83</td>
<td>0</td>
<td>2.01</td>
<td>-0.92</td>
<td>0.26</td>
</tr>
<tr>
<td>0.09</td>
<td>83</td>
<td>0</td>
<td>2.67</td>
<td>-1.16</td>
<td>0.36</td>
</tr>
<tr>
<td>0.1</td>
<td>83</td>
<td>0</td>
<td>3.33</td>
<td>-1.37</td>
<td>0.45</td>
</tr>
</tbody>
</table>

The storage coefficients in layers 2 – 7 are also constant (0.0004). Sensitivity analysis results indicate that the changes of PCE concentrations and MCL arrival time at the WTP caused by variations of storage coefficients are negligible. The results for storage coefficients in layer 2 are summarized in Figure 3.7 and Table 3.3. Results for the remaining layers are similar, and therefore not given out.
Table 3.3. Sensitivity analysis results for storage coefficient in layer 2

<table>
<thead>
<tr>
<th>Storage Coefficient in Layer 2</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>0.00005</td>
<td>83</td>
<td>0</td>
<td>0.01</td>
<td>-0.03</td>
<td>0.00</td>
</tr>
<tr>
<td>0.0001</td>
<td>83</td>
<td>0</td>
<td>0.01</td>
<td>-0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>0.0002</td>
<td>83</td>
<td>0</td>
<td>0.01</td>
<td>-0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>0.0004</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.0006</td>
<td>83</td>
<td>0</td>
<td>0.01</td>
<td>-0.01</td>
<td>0.00</td>
</tr>
<tr>
<td>0.0008</td>
<td>83</td>
<td>0</td>
<td>0.03</td>
<td>-0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>0.001</td>
<td>83</td>
<td>0</td>
<td>0.04</td>
<td>-0.02</td>
<td>0.00</td>
</tr>
<tr>
<td>0.002</td>
<td>83</td>
<td>0</td>
<td>0.10</td>
<td>-0.06</td>
<td>0.01</td>
</tr>
<tr>
<td>0.003</td>
<td>83</td>
<td>0</td>
<td>0.17</td>
<td>-0.09</td>
<td>0.02</td>
</tr>
<tr>
<td>0.004</td>
<td>83</td>
<td>0</td>
<td>0.23</td>
<td>-0.12</td>
<td>0.03</td>
</tr>
<tr>
<td>0.005</td>
<td>83</td>
<td>0</td>
<td>0.30</td>
<td>-0.15</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Figure 3.7. Sensitivity analysis results for storage coefficient in layer 2
3.2.2.2 Hydraulic Conductivities

Hydraulic conductivities are porous medium properties used in the Block-Centered Flow package of MODFLOW simulation. The hydraulic conductivity values read from the BCF file are the horizontal hydraulic conductivities \( K_H, LT^{-1} \) along rows. The hydraulic conductivities along columns are obtained by multiplying \( K_H \) by a ratio, which is 1.0 in the Camp Lejeune model, meaning an isotropic hydraulic conductivity field. This ratio remained unchanged during the sensitivity analysis.

Another hydraulic conductivity related parameter used in the Block-Centered Flow package is leakance, which is calculated by using equation

\[
L_{k,i,j} = \frac{2}{\frac{Z_{k,i,j}}{K_{V(k,i,j)}} + \frac{Z_{k+1,i,j}}{K_{V(k+1,i,j)}}}, \tag{3.5}
\]

where \( k \) is layer number; \( i \) is row number; \( j \) is column number; \( L_{k,i,j} \) is the leakance value at node \( (k,i,j) \) \( (T^{-1}) \); \( Z_{k,i,j} \) is the depth of node \( (k,i,j) \) \( (L) \); and \( K_{V(k,i,j)} \) is the vertical hydraulic conductivity at node \( (k,i,j) \) \( (LT^{-1}) \). Among them, \( K_{V(k,i,j)} \) is obtained as a fraction of \( K_{H(k,i,j)} \), the horizontal hydraulic conductivity at node \( (k,i,j) \) \( (LT^{-1}) \). The ratios of \( K_{H(k,i,j)} \) to \( K_{V(k,i,j)} \) for different layers at the Camp Lejeune site are listed in Table 3.4. These ratios were kept constant as well.

<table>
<thead>
<tr>
<th>Layer</th>
<th>( K_{H(k,i,j)}/K_{V(k,i,j)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.27</td>
</tr>
<tr>
<td>2</td>
<td>10.00</td>
</tr>
<tr>
<td>3</td>
<td>8.26</td>
</tr>
<tr>
<td>4</td>
<td>10.00</td>
</tr>
<tr>
<td>5</td>
<td>10.00</td>
</tr>
<tr>
<td>6</td>
<td>10.00</td>
</tr>
<tr>
<td>7</td>
<td>10.00</td>
</tr>
</tbody>
</table>
During the sensitivity analysis, the horizontal hydraulic conductivities of each layer were varied from -50% to 50%, and the resulting changes of PCE concentrations and MCL arrival times at the WTP were calculated. Some variations of hydraulic conductivities caused appearance of dry wells, and therefore no analysis could be conducted for these variations. The analysis results for the remaining variations are summarized in Figures 3.8 to 3.14, and Tables 3.5 to 3.11.

From the figures and tables, it can be observed that the horizontal hydraulic conductivities in layers 1, 2, and 7 have positive effects on the PCE concentrations at the WTP, which means that an increase in conductivity values can yield higher PCE concentration, while the hydraulic conductivities in layers 3, 4, 5, and 6 cause negative effects. However, as one can see from Tables 3.5 to 3.11, the PCE MCL arrival time at the WTP is not quite sensitive to the change of hydraulic conductivity values in layers 2 – 7, except that the variations in layer 1 cause a change of -14 stress periods in the PCE MCL arrival time.
Figure 3.8. Sensitivity analysis results for hydraulic conductivities in layer 1

Table 3.5. Sensitivity analysis results for hydraulic conductivities in layer 1

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 1 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>79</td>
<td>-4</td>
<td>8.67</td>
<td>0.66</td>
<td>2.38</td>
</tr>
<tr>
<td>20</td>
<td>76</td>
<td>-7</td>
<td>15.54</td>
<td>0.98</td>
<td>4.26</td>
</tr>
<tr>
<td>30</td>
<td>73</td>
<td>-10</td>
<td>20.56</td>
<td>1.09</td>
<td>5.83</td>
</tr>
<tr>
<td>40</td>
<td>71</td>
<td>-12</td>
<td>23.91</td>
<td>0.77</td>
<td>7.21</td>
</tr>
<tr>
<td>50</td>
<td>69</td>
<td>-14</td>
<td>25.89</td>
<td>0.37</td>
<td>8.49</td>
</tr>
</tbody>
</table>
Figure 3.9. Sensitivity analysis results for hydraulic conductivities in layer 2

Table 3.6. Sensitivity analysis results for hydraulic conductivities in layer 2

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 2 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50</td>
<td>86</td>
<td>3</td>
<td>-3.01</td>
<td>-20.07</td>
<td>-16.33</td>
</tr>
<tr>
<td>-30</td>
<td>84</td>
<td>1</td>
<td>-1.99</td>
<td>-10.37</td>
<td>-8.30</td>
</tr>
<tr>
<td>-20</td>
<td>84</td>
<td>1</td>
<td>-1.34</td>
<td>-6.47</td>
<td>-5.14</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>-0.67</td>
<td>-3.04</td>
<td>-2.40</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>82</td>
<td>-1</td>
<td>2.71</td>
<td>0.64</td>
<td>2.13</td>
</tr>
<tr>
<td>20</td>
<td>82</td>
<td>-1</td>
<td>5.15</td>
<td>1.26</td>
<td>4.03</td>
</tr>
<tr>
<td>30</td>
<td>82</td>
<td>-1</td>
<td>7.36</td>
<td>1.86</td>
<td>5.73</td>
</tr>
<tr>
<td>40</td>
<td>82</td>
<td>-1</td>
<td>9.36</td>
<td>2.40</td>
<td>7.28</td>
</tr>
<tr>
<td>50</td>
<td>81</td>
<td>-2</td>
<td>11.19</td>
<td>2.89</td>
<td>8.68</td>
</tr>
</tbody>
</table>
Figure 3.10. Sensitivity analysis results for hydraulic conductivities in layer 3

Table 3.7. Sensitivity analysis results for hydraulic conductivities in layer 3

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 3 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>-30</td>
<td>82</td>
<td>-1</td>
<td>1.44 (-0.09)</td>
<td>0.67</td>
<td>0.68</td>
</tr>
<tr>
<td>-20</td>
<td>82</td>
<td>-1</td>
<td>0.94 (-0.07)</td>
<td>0.43</td>
<td>0.44</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>0.46 (-0.05)</td>
<td>0.21</td>
<td>0.21</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00 (0.00)</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>83</td>
<td>0</td>
<td>0.11 (-0.83)</td>
<td>-0.37</td>
<td>0.39</td>
</tr>
<tr>
<td>20</td>
<td>84</td>
<td>1</td>
<td>0.24 (-1.56)</td>
<td>-0.70</td>
<td>0.74</td>
</tr>
<tr>
<td>30</td>
<td>85</td>
<td>2</td>
<td>0.39 (-2.24)</td>
<td>-0.98</td>
<td>1.07</td>
</tr>
<tr>
<td>40</td>
<td>85</td>
<td>2</td>
<td>0.56 (-2.84)</td>
<td>-1.24</td>
<td>1.37</td>
</tr>
<tr>
<td>50</td>
<td>86</td>
<td>3</td>
<td>0.75 (-3.42)</td>
<td>-1.47</td>
<td>1.66</td>
</tr>
</tbody>
</table>
Figure 3.11. Sensitivity analysis results for hydraulic conductivities in layer 4

Table 3.8. Sensitivity analysis results for hydraulic conductivities in layer 4

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 4 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>-50</td>
<td>82</td>
<td>-1</td>
<td>8.27</td>
<td>5.42</td>
<td>7.02</td>
</tr>
<tr>
<td>-40</td>
<td>82</td>
<td>-1</td>
<td>6.36</td>
<td>4.00</td>
<td>5.41</td>
</tr>
<tr>
<td>-30</td>
<td>82</td>
<td>-1</td>
<td>4.58</td>
<td>2.79</td>
<td>3.90</td>
</tr>
<tr>
<td>-20</td>
<td>82</td>
<td>-1</td>
<td>2.93</td>
<td>1.75</td>
<td>2.50</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>1.41</td>
<td>0.83</td>
<td>1.21</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>83</td>
<td>0</td>
<td>-0.76</td>
<td>-1.31</td>
<td>-1.12</td>
</tr>
<tr>
<td>20</td>
<td>83</td>
<td>0</td>
<td>-1.46</td>
<td>-2.53</td>
<td>-2.17</td>
</tr>
<tr>
<td>30</td>
<td>83</td>
<td>0</td>
<td>-2.11</td>
<td>-3.67</td>
<td>-3.14</td>
</tr>
<tr>
<td>40</td>
<td>84</td>
<td>1</td>
<td>-2.72</td>
<td>-4.75</td>
<td>-4.06</td>
</tr>
<tr>
<td>50</td>
<td>84</td>
<td>1</td>
<td>-3.29</td>
<td>-5.76</td>
<td>-4.92</td>
</tr>
</tbody>
</table>
Figure 3.12. Sensitivity analysis results for hydraulic conductivities in layer 5

Table 3.9. Sensitivity analysis results for hydraulic conductivities in layer 5

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 5 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>-50</td>
<td>81</td>
<td>-2</td>
<td>8.23</td>
<td>5.45</td>
<td>6.74</td>
</tr>
<tr>
<td>-40</td>
<td>81</td>
<td>-2</td>
<td>6.41</td>
<td>4.27</td>
<td>5.27</td>
</tr>
<tr>
<td>-30</td>
<td>82</td>
<td>-1</td>
<td>4.68</td>
<td>3.14</td>
<td>3.86</td>
</tr>
<tr>
<td>-20</td>
<td>82</td>
<td>-1</td>
<td>3.04</td>
<td>2.05</td>
<td>2.52</td>
</tr>
<tr>
<td>-10</td>
<td>82</td>
<td>-1</td>
<td>1.49</td>
<td>1.01</td>
<td>1.23</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>84</td>
<td>1</td>
<td>-1.91</td>
<td>-2.77</td>
<td>-2.32</td>
</tr>
<tr>
<td>20</td>
<td>84</td>
<td>1</td>
<td>-3.69</td>
<td>-5.31</td>
<td>-4.46</td>
</tr>
<tr>
<td>30</td>
<td>85</td>
<td>2</td>
<td>-5.36</td>
<td>-7.63</td>
<td>-6.46</td>
</tr>
<tr>
<td>40</td>
<td>86</td>
<td>3</td>
<td>-6.92</td>
<td>-9.79</td>
<td>-8.33</td>
</tr>
<tr>
<td>50</td>
<td>86</td>
<td>3</td>
<td>-8.39</td>
<td>-11.79</td>
<td>-10.08</td>
</tr>
</tbody>
</table>
Figure 3.13. Sensitivity analysis results for hydraulic conductivities in layer 6

Table 3.10. Sensitivity analysis results for hydraulic conductivities in layer 6

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 6 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50</td>
<td>83</td>
<td>0</td>
<td>1.13                          0.70</td>
<td>0.87</td>
<td>0.87</td>
</tr>
<tr>
<td>-40</td>
<td>83</td>
<td>0</td>
<td>0.84                          0.53</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>-30</td>
<td>83</td>
<td>0</td>
<td>0.59                          0.37</td>
<td>0.47</td>
<td>0.47</td>
</tr>
<tr>
<td>-20</td>
<td>83</td>
<td>0</td>
<td>0.37                          0.23</td>
<td>0.29</td>
<td>0.29</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>0.18                          0.11</td>
<td>0.14</td>
<td>0.14</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00                          0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>83</td>
<td>0</td>
<td>-0.10                         -0.17</td>
<td>-0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>20</td>
<td>83</td>
<td>0</td>
<td>-0.19                         -0.33</td>
<td>-0.24</td>
<td>0.24</td>
</tr>
<tr>
<td>30</td>
<td>83</td>
<td>0</td>
<td>-0.26                         -0.49</td>
<td>-0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>40</td>
<td>83</td>
<td>0</td>
<td>-0.34                         -0.65</td>
<td>-0.45</td>
<td>0.45</td>
</tr>
<tr>
<td>50</td>
<td>83</td>
<td>0</td>
<td>-0.40                         -0.81</td>
<td>-0.54</td>
<td>0.54</td>
</tr>
</tbody>
</table>
Figure 3.14. Sensitivity analysis results for hydraulic conductivities in layer 7

Table 3.11. Sensitivity analysis results for hydraulic conductivities in layer 7

<table>
<thead>
<tr>
<th>Increment of $K_H$ in Layer 7 (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>83</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-50</td>
<td>83</td>
<td>0</td>
<td>2.76</td>
<td>-1.51</td>
<td>1.67</td>
</tr>
<tr>
<td>-40</td>
<td>83</td>
<td>0</td>
<td>2.18</td>
<td>-1.20</td>
<td>1.33</td>
</tr>
<tr>
<td>-30</td>
<td>83</td>
<td>0</td>
<td>1.61</td>
<td>-0.89</td>
<td>0.99</td>
</tr>
<tr>
<td>-20</td>
<td>83</td>
<td>0</td>
<td>1.06</td>
<td>-0.59</td>
<td>0.65</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>0.52</td>
<td>-0.29</td>
<td>0.32</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>83</td>
<td>0</td>
<td>0.53</td>
<td>0.28</td>
<td>0.31</td>
</tr>
<tr>
<td>20</td>
<td>83</td>
<td>0</td>
<td>1.05</td>
<td>0.55</td>
<td>0.61</td>
</tr>
<tr>
<td>30</td>
<td>83</td>
<td>0</td>
<td>1.54</td>
<td>0.81</td>
<td>0.90</td>
</tr>
<tr>
<td>40</td>
<td>83</td>
<td>0</td>
<td>2.02</td>
<td>1.07</td>
<td>1.18</td>
</tr>
<tr>
<td>50</td>
<td>83</td>
<td>0</td>
<td>2.48</td>
<td>1.31</td>
<td>1.44</td>
</tr>
</tbody>
</table>
3.2.2.3 Recharge Rate

Recharge rate \((r, \text{LT}^{-1})\) is used in the Recharge package of MODFLOW simulation. In the Camp Lejeune model, the recharge rate is constant for each calendar year, and the values vary between 0.0015 – 0.0044 ft/day through the simulated time period. During the sensitivity analysis, the recharge rate of each stress period is changed from -20\% to 14\%.

As indicated by the results summarized in Figure 3.15 and Table 3.12, increase of recharge rate can cause higher PCE concentrations at the WTP. The variation of the relative change of PCE concentration at the WTP is from -23.93\% to 18.73\%, and the average value of relative changes is about the same as the increase of recharge rate in percentage.

Another observation from Table 3.12 is that, although the PCE concentrations during POI are quite sensitive to the change of recharge rate, variation of recharge rate does not cause much change in the PCE MCL arrival time – a 20\% reduction in recharge rate would cause only one stress period delay in PCE MCL arrival time.

<table>
<thead>
<tr>
<th>Increment of Recharge Rate (%)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td>82</td>
<td>-1</td>
<td>6.92</td>
<td>-23.93</td>
<td>-18.40</td>
</tr>
<tr>
<td>-10</td>
<td>83</td>
<td>0</td>
<td>3.73</td>
<td>-13.12</td>
<td>-9.76</td>
</tr>
<tr>
<td>-5</td>
<td>83</td>
<td>0</td>
<td>1.61</td>
<td>-5.50</td>
<td>-4.24</td>
</tr>
<tr>
<td>0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5</td>
<td>83</td>
<td>0</td>
<td>5.55</td>
<td>-1.51</td>
<td>4.21</td>
</tr>
<tr>
<td>10</td>
<td>83</td>
<td>0</td>
<td>13.61</td>
<td>-3.05</td>
<td>9.79</td>
</tr>
<tr>
<td>14</td>
<td>83</td>
<td>0</td>
<td>18.73</td>
<td>-4.08</td>
<td>13.25</td>
</tr>
</tbody>
</table>
3.2.2.4 First Order Reaction Rate

First order reaction rate \( (k, \ T^{-1}) \) is a chemical property of the contaminant applied in the Chemical Reaction package of MT3DMS. The first order reaction rate of PCE is set to be 5.0\times10^{-4}/day for the Camp Lejeune model. Ten reactions rates were evenly selected within the range of 2.3\times10^{-4} – 7.7\times10^{-4}/day during the sensitivity analysis.

The analysis results shown in Figure 3.16 and Table 3.13 indicate that the first order reaction rate is one of the most critical uncertain variables that can cause negative changes of the PCE concentrations at the WTP during POI. Variations of the first order reaction rate between 2.3\times10^{-4} – 7.7\times10^{-4}/day can cause -37.96% – 69.84% relative PCE concentration changes. Interestingly, although variation of first order reaction rate can
cause significant change in the PCE concentrations, the PCE MCL arrival time at the WTP is not affected too much – it only varies between -1 – 1 stress period.

Figure 3.16. Sensitivity analysis results for first order reaction rate

<table>
<thead>
<tr>
<th>Reaction Rate (1/day)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00023</td>
<td>82</td>
<td>-1</td>
<td>69.84</td>
<td>51.79</td>
<td>51.79</td>
</tr>
<tr>
<td>0.000284</td>
<td>82</td>
<td>-1</td>
<td>52.10</td>
<td>39.39</td>
<td>39.39</td>
</tr>
<tr>
<td>0.000338</td>
<td>82</td>
<td>-1</td>
<td>36.52</td>
<td>28.11</td>
<td>28.11</td>
</tr>
<tr>
<td>0.000392</td>
<td>82</td>
<td>-1</td>
<td>22.80</td>
<td>17.86</td>
<td>17.86</td>
</tr>
<tr>
<td>0.000446</td>
<td>83</td>
<td>0</td>
<td>10.70</td>
<td>8.51</td>
<td>8.51</td>
</tr>
<tr>
<td>0.0005</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.000554</td>
<td>83</td>
<td>0</td>
<td>-6.90</td>
<td>-7.78</td>
<td>7.78</td>
</tr>
<tr>
<td>0.000608</td>
<td>83</td>
<td>0</td>
<td>-13.32</td>
<td>-14.88</td>
<td>14.88</td>
</tr>
<tr>
<td>0.000662</td>
<td>84</td>
<td>1</td>
<td>-19.27</td>
<td>-21.37</td>
<td>21.37</td>
</tr>
<tr>
<td>0.000716</td>
<td>84</td>
<td>1</td>
<td>-24.79</td>
<td>-27.31</td>
<td>27.31</td>
</tr>
<tr>
<td>0.00077</td>
<td>84</td>
<td>1</td>
<td>-29.92</td>
<td>-32.75</td>
<td>32.75</td>
</tr>
</tbody>
</table>
3.2.2.5 Distribution Coefficient

Distribution coefficient \((K_d, \text{L}^3\text{M}^{-1})\) is a contaminant property in the Chemical Reaction package of MT3DMS simulation. In the Camp Lejeune model, the value of distribution coefficient is a constant of \(5.0 \times 10^{-6} \text{ ft}^3/\text{g}\). During the sensitivity analysis, the distribution coefficient values were evenly selected within the range of \(1.77 \times 10^{-6} – 2.43 \times 10^{-5} \text{ ft}^3/\text{g}\).

Analysis results in Figure 3.17 and Table 3.14 indicate that the PCE concentrations and MCL arrival time are very sensitive to the change of distribution coefficient. Variation of distribution coefficient cause negative change to PCE concentration, and the relative change varies between -99.49% and 37.07%. According to the analysis results, increasing the distribution coefficient to \(2.43 \times 10^{-5} \text{ ft}^3/\text{g}\) would cause a 218-month delay in the PCE MCL arrival time.

Figure 3.17. Sensitivity analysis results for distribution coefficient
### Table 3.14. Sensitivity analysis results for distribution coefficient

<table>
<thead>
<tr>
<th>Distribution Coefficient (f/ft³)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.77 x 10⁻⁶</td>
<td>58</td>
<td>-25</td>
<td>37.07 - 7.22</td>
<td>14.00</td>
<td>16.42</td>
</tr>
<tr>
<td>4.27 x 10⁻⁶</td>
<td>77</td>
<td>-6</td>
<td>8.16 - 0.14</td>
<td>2.95</td>
<td>2.97</td>
</tr>
<tr>
<td>5.00 x 10⁻⁶</td>
<td>83</td>
<td>0</td>
<td>0.00 - 0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>6.78 x 10⁻⁶</td>
<td>96</td>
<td>13</td>
<td>-3.27 - 19.21</td>
<td>-8.67</td>
<td>8.67</td>
</tr>
<tr>
<td>1.18 x 10⁻⁵</td>
<td>144</td>
<td>61</td>
<td>-30.42 - 69.72</td>
<td>-42.46</td>
<td>42.46</td>
</tr>
<tr>
<td>1.43 x 10⁻⁵</td>
<td>180</td>
<td>97</td>
<td>-42.29 - 85.37</td>
<td>-58.52</td>
<td>58.52</td>
</tr>
<tr>
<td>1.68 x 10⁻⁵</td>
<td>219</td>
<td>136</td>
<td>-53.46 - 93.43</td>
<td>-71.32</td>
<td>71.32</td>
</tr>
<tr>
<td>1.93 x 10⁻⁵</td>
<td>250</td>
<td>167</td>
<td>-63.56 - 97.14</td>
<td>-80.74</td>
<td>80.74</td>
</tr>
<tr>
<td>2.18 x 10⁻⁵</td>
<td>279</td>
<td>196</td>
<td>-72.32 - 98.79</td>
<td>-87.33</td>
<td>87.33</td>
</tr>
<tr>
<td>2.43 x 10⁻⁵</td>
<td>301</td>
<td>218</td>
<td>-79.58 - 99.49</td>
<td>-91.80</td>
<td>91.80</td>
</tr>
</tbody>
</table>

#### 3.2.2.6 Mass Loading Rate

Mass loading rate \((m, \text{MT}^{-1})\) is the releasing rate of contaminant to the groundwater system, which is a parameter contained in the Sink & Source Mixing package. For the Camp Lejeune model, the PCE is assumed to be released to the Tarawa Terrace groundwater system at a constant rate of 1,200 g/day. According to the historical records, the actual releasing rate varied between 200 – 2,200 g/day. Therefore, 10 mass loading rates were selected within this range for the sensitivity analysis.

From the analysis results presented in Figure 3.18 and Table 3.15, it can be seen that the effect of mass loading rate variation to the PCE concentration at the WTP is positive and linear – a 10% increase of mass loading rate would cause exactly a 10% increase of the PCE concentration at the WTP. The PCE MCL arrival time is also quite sensitive to the change of mass loading rate (-5 – 20 stress periods), but the effect is no...
longer linear - reduction of mass loading rate can cause more change in the PCE MCL arrival time than that can be caused by the same amount of increment.

Figure 3.18. Sensitivity analysis results for mass loading rate

Table 3.15. Sensitivity analysis results for mass loading rate

<table>
<thead>
<tr>
<th>Mass Loading Rate (g/day)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>103</td>
<td>20</td>
<td>-83.33</td>
<td>-83.33</td>
<td>-83.33</td>
</tr>
<tr>
<td>400</td>
<td>93</td>
<td>10</td>
<td>-66.67</td>
<td>-66.67</td>
<td>-66.67</td>
</tr>
<tr>
<td>600</td>
<td>89</td>
<td>6</td>
<td>-50.00</td>
<td>-50.00</td>
<td>-50.00</td>
</tr>
<tr>
<td>800</td>
<td>86</td>
<td>3</td>
<td>-33.33</td>
<td>-33.34</td>
<td>-33.34</td>
</tr>
<tr>
<td>1,000</td>
<td>84</td>
<td>1</td>
<td>-16.66</td>
<td>-16.68</td>
<td>-16.67</td>
</tr>
<tr>
<td>1,200</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1,400</td>
<td>82</td>
<td>-1</td>
<td>16.67</td>
<td>16.65</td>
<td>16.66</td>
</tr>
<tr>
<td>1,600</td>
<td>81</td>
<td>-2</td>
<td>33.34</td>
<td>33.32</td>
<td>33.33</td>
</tr>
<tr>
<td>1,800</td>
<td>80</td>
<td>-3</td>
<td>50.00</td>
<td>49.99</td>
<td>49.99</td>
</tr>
<tr>
<td>2,000</td>
<td>79</td>
<td>-4</td>
<td>66.67</td>
<td>66.65</td>
<td>66.66</td>
</tr>
<tr>
<td>2,200</td>
<td>78</td>
<td>-5</td>
<td>83.33</td>
<td>83.32</td>
<td>83.32</td>
</tr>
</tbody>
</table>
3.2.2.7 Bulk Density

Bulk density ($\rho_b$, ML$^{-3}$) is an aquifer medium property presented in the Chemical Reaction package of MT3DMS simulation. A constant value of 77,112 g/ft$^3$ is used for all the cells in the Camp Lejeune model. During the sensitivity analysis process, 10 values were evenly picked up within the range of 69,943 – 78,098 g/ft$^3$. The simulation results are summarized in Figure 3.19 and Table 3.16. According to the simulation results, increasing of bulk density causes negative effects to the PCE concentrations at the WTP, while decreasing of bulk density can shorten the PCE MCL arrival time. The changes caused by the variation of bulk density are relatively small (-0.74% – 5.27% relative change of PCE concentrations and -4 – 0 stress periods change of PCE MCL arrival time) compared to changes caused by other uncertain variables such as mass loading rate.

Figure 3.19. Sensitivity analysis results for bulk density
Table 3.16. Sensitivity analysis results for bulk density

<table>
<thead>
<tr>
<th>Bulk Density (g/ft$^3$)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>69,943</td>
<td>79</td>
<td>-4</td>
<td>5.27</td>
<td>1.91</td>
<td>1.91</td>
</tr>
<tr>
<td>70,849</td>
<td>80</td>
<td>-3</td>
<td>4.60</td>
<td>1.67</td>
<td>1.67</td>
</tr>
<tr>
<td>71,755</td>
<td>80</td>
<td>-3</td>
<td>3.94</td>
<td>1.44</td>
<td>1.44</td>
</tr>
<tr>
<td>72,661</td>
<td>81</td>
<td>-2</td>
<td>3.28</td>
<td>1.20</td>
<td>1.20</td>
</tr>
<tr>
<td>73,567</td>
<td>81</td>
<td>-2</td>
<td>2.62</td>
<td>0.96</td>
<td>0.96</td>
</tr>
<tr>
<td>74,474</td>
<td>82</td>
<td>-1</td>
<td>1.95</td>
<td>0.71</td>
<td>0.71</td>
</tr>
<tr>
<td>75,380</td>
<td>82</td>
<td>-1</td>
<td>1.28</td>
<td>0.47</td>
<td>0.47</td>
</tr>
<tr>
<td>76,286</td>
<td>82</td>
<td>-1</td>
<td>0.61</td>
<td>0.22</td>
<td>0.22</td>
</tr>
<tr>
<td>77,112</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>77,192</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>-0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>78,098</td>
<td>83</td>
<td>0</td>
<td>-0.04</td>
<td>-0.28</td>
<td>0.28</td>
</tr>
</tbody>
</table>

3.2.2.8 Longitudinal Dispersivity

Longitudinal dispersivity ($\alpha_L$, L) is a property of the porous medium as described in the Dispersion package of MT3DMS model. Along with longitudinal dispersivity, the Dispersion package also defines the ratios of the horizontal transverse dispersivity ($\alpha_{TH}$) and vertical transverse dispersivity ($\alpha_{TV}$) to the longitudinal dispersivity. During the sensitivity analysis process in this study, these ratios remain unaltered. The longitudinal dispersivity value in the Camp Lejeune model is constant – 25 ft for each cell. The range of variation used in the sensitivity analysis is 2.5 ft – 125 ft (0.1$\alpha_L$ – 5.0$\alpha_L$). Within the range of variation, a total number of 16 simulations were conducted.

From the analysis results summarized in Table 3.17 and Figure 3.20, it can be observed that even with a change of 400% to the $\alpha_L$ values, the average of absolute relative change for the PCE concentration at the WTP is only 6.71%, which can be taken as negligible. However, the significant changes of PCE MCL arrival time (-20 stress
periods – 10 stress periods) indicate that the PCE MCL arrival time is very sensitive to the change of the longitudinal dispersivity value, and the increasing of the longitudinal dispersivity would shorten the PCE MCL arrival time at the WTP.

Table 3.17. Sensitivity analysis results for longitudinal dispersivity

<table>
<thead>
<tr>
<th>Longitudinal Dispersivity (ft)</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>93</td>
<td>10</td>
<td>4.93</td>
<td>-8.29</td>
<td>-2.44</td>
</tr>
<tr>
<td>5.0</td>
<td>92</td>
<td>9</td>
<td>4.29</td>
<td>-7.19</td>
<td>-2.09</td>
</tr>
<tr>
<td>10.0</td>
<td>89</td>
<td>6</td>
<td>3.07</td>
<td>-5.15</td>
<td>-1.47</td>
</tr>
<tr>
<td>15.0</td>
<td>87</td>
<td>4</td>
<td>1.95</td>
<td>-3.30</td>
<td>-0.92</td>
</tr>
<tr>
<td>20.0</td>
<td>85</td>
<td>2</td>
<td>0.93</td>
<td>-1.59</td>
<td>-0.43</td>
</tr>
<tr>
<td>25.0</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>30.0</td>
<td>81</td>
<td>-2</td>
<td>1.47</td>
<td>-0.86</td>
<td>0.38</td>
</tr>
<tr>
<td>40.0</td>
<td>78</td>
<td>-5</td>
<td>4.11</td>
<td>-2.36</td>
<td>1.01</td>
</tr>
<tr>
<td>50.0</td>
<td>75</td>
<td>-8</td>
<td>6.39</td>
<td>-3.67</td>
<td>1.51</td>
</tr>
<tr>
<td>60.0</td>
<td>73</td>
<td>-10</td>
<td>8.38</td>
<td>-4.79</td>
<td>1.90</td>
</tr>
<tr>
<td>70.0</td>
<td>71</td>
<td>-12</td>
<td>10.14</td>
<td>-5.77</td>
<td>2.20</td>
</tr>
<tr>
<td>80.0</td>
<td>69</td>
<td>-14</td>
<td>11.70</td>
<td>-6.63</td>
<td>2.44</td>
</tr>
<tr>
<td>90.0</td>
<td>68</td>
<td>-15</td>
<td>13.09</td>
<td>-7.39</td>
<td>2.62</td>
</tr>
<tr>
<td>100.0</td>
<td>66</td>
<td>-17</td>
<td>14.36</td>
<td>-8.07</td>
<td>2.77</td>
</tr>
<tr>
<td>110.0</td>
<td>65</td>
<td>-18</td>
<td>15.49</td>
<td>-8.68</td>
<td>2.87</td>
</tr>
<tr>
<td>125.0</td>
<td>63</td>
<td>-20</td>
<td>16.99</td>
<td>-9.49</td>
<td>2.97</td>
</tr>
</tbody>
</table>
3.2.2.9 Effective Porosity

Effective porosity ($\theta$) is described in the Basic Transport package of MT3DMS simulation. It is the ratio of pore spaces that are effective for the groundwater flow over the bulk volume of the porous medium. For the Camp Lejeune model, the effective porosities in all the cells are assigned to be 0.20. During the sensitivity analysis, 10 values were selected within the range of 0.10 – 0.30 for contaminant transport simulations. As indicated in Figure 3.21 and Table 3.18, variations of the effective porosity values can cause obvious changes in the PCE concentrations (-42.29% – 95.41%) and PCE MCL arrival time (-11 stress periods – 11 stress periods) at the WTP. A positive change to the effective porosity would cause a reduction in PCE concentration and a delay in the PCE MCL arrival time.
Figure 3.21. Sensitivity analysis results for effective porosity

Table 3.18. Sensitivity analysis results for effective porosity

<table>
<thead>
<tr>
<th>Effective Porosity</th>
<th>MCL Arrival Time (SP)</th>
<th>Change of MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP</th>
<th>Mean of Relative Change</th>
<th>Mean of Absolute Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Max.</td>
<td>Min.</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>72</td>
<td>-11</td>
<td>95.41</td>
<td>47.63</td>
<td>58.34</td>
</tr>
<tr>
<td>0.12</td>
<td>74</td>
<td>-9</td>
<td>68.90</td>
<td>36.33</td>
<td>43.64</td>
</tr>
<tr>
<td>0.14</td>
<td>76</td>
<td>-7</td>
<td>46.91</td>
<td>26.02</td>
<td>30.72</td>
</tr>
<tr>
<td>0.16</td>
<td>79</td>
<td>-4</td>
<td>28.54</td>
<td>16.59</td>
<td>19.29</td>
</tr>
<tr>
<td>0.18</td>
<td>81</td>
<td>-2</td>
<td>13.08</td>
<td>7.95</td>
<td>9.11</td>
</tr>
<tr>
<td>0.20</td>
<td>83</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.22</td>
<td>85</td>
<td>2</td>
<td>-7.33</td>
<td>-11.15</td>
<td>-8.20</td>
</tr>
<tr>
<td>0.24</td>
<td>87</td>
<td>4</td>
<td>-14.08</td>
<td>-20.70</td>
<td>-15.60</td>
</tr>
<tr>
<td>0.26</td>
<td>90</td>
<td>7</td>
<td>-20.30</td>
<td>-28.92</td>
<td>-22.30</td>
</tr>
<tr>
<td>0.28</td>
<td>91</td>
<td>8</td>
<td>-26.04</td>
<td>-36.05</td>
<td>-28.39</td>
</tr>
<tr>
<td>0.30</td>
<td>94</td>
<td>11</td>
<td>-31.35</td>
<td>-42.29</td>
<td>-33.93</td>
</tr>
</tbody>
</table>
3.2.2.10 Summary of Sensitivity Analysis Results

The sensitivity analysis results regarding all the uncertain variables discussed in this chapter are summarized in Table 3.19. In the table, the ranges of change for PCE MCL arrival times and relative change of PCE concentrations at the WTP caused by the variations of uncertain parameters are given in columns two and three, respectively.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Change of PCE MCL Arrival Time (SP)</th>
<th>Relative Change of PCE Concentration at the WTP (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific Storage of Layer 1</td>
<td>0</td>
<td>-2.78 – 3.33</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 2</td>
<td>0</td>
<td>-0.15 – 0.3</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 3</td>
<td>0</td>
<td>-0.13 – 0.26</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 4</td>
<td>0</td>
<td>-0.15 – 0.24</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 5</td>
<td>0</td>
<td>-0.10 – 0.22</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 6</td>
<td>0</td>
<td>-0.10 – 0.21</td>
</tr>
<tr>
<td>Storage Coefficient of Layer 7</td>
<td>0</td>
<td>-0.10 – 0.21</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 1</td>
<td>-4 – -14</td>
<td>0.37 – 25.89</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 2</td>
<td>-2 – 3</td>
<td>-20.07 – 11.19</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 3</td>
<td>-1 – 3</td>
<td>-3.42 – 1.44</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 4</td>
<td>-1 – 1</td>
<td>-5.76 – 8.27</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 5</td>
<td>-2 – 3</td>
<td>-11.79 – 8.23</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 6</td>
<td>0</td>
<td>-0.81 – 1.13</td>
</tr>
<tr>
<td>Horizontal Hydraulic Conductivity of Layer 7</td>
<td>0</td>
<td>-2.88 – 2.76</td>
</tr>
<tr>
<td>Recharge Rate</td>
<td>-1 – 0</td>
<td>-23.93 – 18.73</td>
</tr>
<tr>
<td>First Order Reaction Rate</td>
<td>-1 – 0</td>
<td>-37.96 – 69.84</td>
</tr>
<tr>
<td>Distribution Coefficient</td>
<td>-25 – 237</td>
<td>-99.78 – 37.07</td>
</tr>
<tr>
<td>Mass Loading Rate</td>
<td>-5 – 20</td>
<td>-83.33 – 83.33</td>
</tr>
<tr>
<td>Bulk Density</td>
<td>-4 – 1</td>
<td>-1.41 – 1.91</td>
</tr>
<tr>
<td>Effective Porosity</td>
<td>-11 – 11</td>
<td>-42.29 – 95.41</td>
</tr>
</tbody>
</table>

From Table 3.19, it can be observed that the PCE MCL arrival time at the WTP is most sensitive to changes of distribution coefficient, longitudinal dispersivity, mass...
loading rate, effective porosity, and hydraulic conductivities in layer 1, while the PCE
concentrations at the WTP are most sensitive to mass loading rate, effective porosity,
distribution coefficient, first order reaction rate, and recharge rate. Therefore, the
following parameters are selected as the critical uncertain variables that will be applied in
the followed uncertainty analysis:

i. Hydraulic conductivities in layer 1;
ii. Effective porosity;
iii. First order reaction rate;
iv. Mass loading rate;
v. Recharge rate;
vi. Distribution coefficient; and
vii. Longitudinal dispersivity.

Besides the critical variables mentioned above, considering the fact that stochastic
distributions of heterogenous parameters may cause significant change to the PCE
concentrations and MCL arrival times at the WTP, bulk density and hydraulic
conductivities in layers 3 and 5 are also added to the critical uncertain variables list.

3.3 Summary

Exposures of human beings to environmental contaminants might cause serious
health effects. Epidemiologic study is a method used by health scientists to reveal their
relationships. In retrospective epidemiologic studies, quantitative historical information is
often too limited for an exposure assessment. One way to fill the data gap is historical
reconstruction and simulation analyses [Maslia et al., 2003; Nieuwenhuijsen et al., 2006].

In this chapter, the historical reconstructions of contaminant exposure levels for an
epidemiologic study conducted at U.S. Marine Corps Base Camp Lejeune, North Carolina by ATSDR are introduced.

Due to the nature of the historical reconstruction process, there are often uncertainties associated with the input data, and therefore, the output of the simulation models, which may seriously impact the related epidemiologic investigations. One way to evaluate the uncertainties residing in the final simulation results is uncertainty analysis. Due to the numerous uncertain parameters used in the Camp Lejeune model, sensitivity analyses to these uncertain variables prior to the uncertainty analysis, which can screen out the most critical variables for the uncertainty analysis, are necessary for an efficient and reliable uncertainty analysis.

In this chapter, the sensitivities of the uncertain parameters were evaluated from two aspects: the PCE MCL arrival time and the PCE concentrations at the WTP. For each uncertain parameter, several values were picked up within its nominal range, and groundwater flow and contaminant fate-and-transport were simulated by using these values. The relative changes of PCE MCL arrival time and contaminant concentrations were then calculated and compared. According to the sensitivity analyses results, the following parameters are selected as the critical uncertain variables for the followed uncertainty analysis:

i. Hydraulic conductivities in aquifer layers 1, 3, and 5;
ii. Effective porosity;
iii. First order reaction rate;
iv. Mass loading rate;
v. Recharge rate;
vi. Bulk density;

vii. Distribution coefficient; and

viii. Longitudinal dispersivity.
CHAPTER 4

EFFECT OF PUMPING SCHEDULE VARIATION ON CONTAMINANT CONCENTRATIONS AND ARRIVAL TIMES

Among all the input parameters that might take uncertainties into the final simulation results of the Camp Lejeune model, pumping schedule is very unique in that it causes uncertainties through two different pathways – the MODFLOW simulation and the volumetric mixing model. To evaluate the effect of pumping schedule uncertainties, a simple sensitivity analysis as introduced in Chapter 3 may not be sufficient because, as it is well known, manipulation of the pumping schedule may cause dramatic change in the groundwater flow as well as contaminant fate and transport in a subsurface system. Thus, in this chapter we evaluate the effect of pumping schedule variation on contaminant concentration and arrival time without considering other uncertain parameters. To quantify this effect, pumping schedules are optimized and used as input in groundwater flow and contaminant transport simulation models to obtain extreme arrival times (i.e., earliest and latest arrival times) and a range of possible arrival times in between. During a groundwater contamination event, the contaminant concentration at the exposure point would gradually increase to the specified exposure level. Therefore, optimization of the pumping schedule for extreme contaminant arrival time is equivalent to optimizing the pumping schedule for maximum or minimum contaminant concentration in the delivered water.

Numerous studies exist in the literature regarding pumping schedules optimization, largely due to the intensive research of remediation scheme optimization problems [Cunha, 2002; Das and Datta, 2001; Freeze and Gorelick, 1999; Gorelick,
In the past two decades, a variety of optimization methods have been proposed to optimize the remediation policies, including the pumping rates and locations of pumping wells. These methods can be separated into two categories: classical mathematical programming methods and heuristic methods. Examples of classical mathematical programming methods include linear programming (LP) [Atwood and Gorelick, 1985], nonlinear programming (NLP) [Ahlfeld et al., 1988a, b; Bear and Sun, 1998; Gorelick et al., 1984; Wagner and Gorelick, 1987; Wang and Ahlfeld, 1994], control theory algorithms [Chang et al., 1992; Culver and Shoemaker, 1992, 1993, 1997; Culver and Shenk, 1998], and successive approximation methods [Karatzas and Pinder, 1993; 1996]. The most popular heuristic methods are genetic algorithms (GAs), simulated annealing (SA), and tabu search (TS) [Reeves, 1996]. GAs have been applied in works of Rogers and Dowla [1994], McKinney and Lin [1994], Rogers et al. [1995], Huang and Mayer [1997], Guan and Aral [1999]; SA methods have been used by Dougherty and Marryott [1991], Kuo et al. [1992], Marryott et al. [1993], Rizzo and Dougherty [1996], Wang and Zheng [1998a], Skaggs et al. [2001], Rao et al. [2003]; and Zheng and Wang [1999b] used TS method to find the optimal pumping schemes for hydraulic containment problems. Although each of the above optimization methods has its own advantages and disadvantages, one common limitation of all of the above methods is that the application of these methods to field-scale problems is very limited due to high computational demands [Zheng and Wang, 2002]. Considering that the simulations models constructed for most epidemiologic studies are for large-scale and complex systems, the focus of this chapter is the development of an efficient and reliable pumping schedule optimization procedure that can be applied to field-scale problems.
This procedure is referred to as the Pumping Schedule Optimization System (PSOpS). For a generic application of the procedure, PSOpS assumes a dynamic pumping schedule, and the basic time unit for pumping schedule optimization is a “stress period” as used in MODFLOW and MT3DMS simulations. For each stress period, the pumping rates in water-supply wells are optimized while the total pumping demand is assumed to be constant. Two improved nonlinear programming methods – Rank-and-Assign (RAA) and Improved Gradient (IG) – are used in PSOpS to provide computational efficiency. The efficiency and reliability of PSOpS were tested using a simple example problem and then applied to the Camp Lejuene model.

4.1 Optimization Problem

Evaluation of the changes in contaminant arrival time caused by pumping schedule variations requires optimal pumping schedules that can yield extreme contaminant arrival times. This is analogous to optimizing the pumping schedules for maximum or minimum contaminant concentration at the exposure point, which can be more easily realized due to the existence of numerous contaminant transport simulation models.

To obtain the extreme (minimum or maximum) contaminant arrival time at an exposure point, an ideal approach would be the optimization of the contaminant concentration at the exposure point for every stress period in sequence until the specific concentration level is exceeded. For the optimization of contaminant concentration at each stress period, decision variables include pumping schedules for the current and all previous stress periods. However, this approach can quickly become computationally infeasible as the number of stress periods increases, especially for a field-scale system.
A sequential multistage optimization approach [Zheng and Wang, 2002] is chosen to formulate the optimization problem in a computationally efficient way. Beginning with the first stress period, the pumping schedule of each stress period is optimized in sequence for the maximum or minimum contaminant concentration at that period, while the piezometric head and contaminant concentration distribution obtained through the optimization of the pumping schedule of previous stress period are used as initial condition. The process continues until the specific contaminant concentration in the delivered water is met. By formulating the optimization problem in this manner, the dimensions of the problem would not increase as the number of stress periods increases, thus the computational demand would only increase linearly.

The optimization model for maximum contaminant concentration within a stress period can be expressed as:

\[
\begin{align*}
\text{Max } C_i &= f(q_1, \ldots, q_i) \\
\text{s.t.} \\
0 &\leq q_i \leq w_i, \\
\sum_{j=1}^{n} q_{ij} &= Q_{Ti} \\
q_k &= q_k^* (k = 1, \ldots, i-1)
\end{align*}
\]

in which \( C_i \) is the contaminant concentration at stress period \( i \) (ML\(^3\)); \( n \) is the total number of active water-supply wells in stress period \( i \); \( q_{ij} \) is the pumping rate of well \( j \) at stress period \( i \) (L\(^3\)T\(^{-1}\)); \( q_i \) is an \( n \)-dimensional vector of pumping rates at stress period \( i \) consists of \( q_{ij} \) (L\(^3\)T\(^{-1}\)); \( w_i \) is an \( n \)-dimensional vector of the upper bound of \( q_i \) at stress period \( i \) (pumping capacities) (L\(^3\)T\(^{-1}\)); \( Q_{Ti} \) is the total water demand at stress period \( i \) (L\(^3\)T\(^{-1}\)); and \( q_k^* \) is the optimal pumping schedules for stress period \( k \) (L\(^3\)T\(^{-1}\)). The optimization formulation for minimum contaminant concentration is equivalent to the
maximization of the negative concentration value in the objective function. Therefore, in this chapter only the “maximization” problem is discussed, but the method provided can be extended to a “minimization” problem easily.

### 4.2 Methodology of PSOpS

PSOpS is a procedure that optimizes pumping schedules for optimum contaminant concentration via a simulation/optimization (S/O) approach – a combinational use of simulation models and optimization techniques. During a PSOpS application, simulators are used to provide contaminant concentration information, and optimizers update the pumping schedule according to the simulation results.

In PSOpS the contaminant concentration in the exposure point is calculated by assuming a volumetric mixing model:

\[
C_i = \frac{\sum_{j=1}^{n} q_j c_{ij}}{Q_{ti}},
\]

(4.2)

where \(c_{ij}\) is the contaminant concentration in pumping well \(j\) at stress period \(i\) (ML\(^{-3}\)). The contaminant concentration \(c_{ij}\) can be obtained from various groundwater flow as well as contaminant fate-and-transport simulation models, such as ISOQUAD [Pinder, 1979] and SUTRA [Voss, 1984]. In PSOpS, the transient contaminant transport is simulated by MT3DMS. The pore velocities used in MT3DMS simulation are calculated according to the piezometric head distribution of the subsurface system, which is provided in PSOpS by the three dimensional groundwater-flow model MODFLOW. Selection of MODFLOW and MT3DMS as simulators is attributed to their popularities. Another benefit for this particular study is that the original input files obtained from the Camp
Lejeune model can be applied directly and only a few complementary files need to be added within the PSOpS framework.

The contaminant transport process in a groundwater system is usually nonlinear. Thus, the optimization formulation in Equation (4.1) is usually a nonlinear optimization problem. Solution of nonlinear optimization problems typically requires repetitive, computationally-expensive evaluation of the objective functions. To reduce the computational demand in solving the nonlinear optimization problem, two optimization techniques are developed and applied in PSOpS – the Rank-and-Assign (RAA) method and the Improved Gradient (IG) method.

The working procedure of PSOpS is described in Figure 4.1. As illustrated, for each stress period, the input data is read first. The pumping schedule of the current stress period is then optimized by the RAA method unless the total pumping demand is zero, which indicates no update is necessary. If the RAA method converges, optimum pumping schedule for the current stress period has been obtained; otherwise the schedule is updated by the IG method. This procedure is repeated till the last stress period in the simulation models. The detailed algorithms of RAA and IG are explained as follows.

![Flowchart of PSOpS](image-url)
4.2.1 Rank-and-Assign Method

With the ability to converge within usually two iterations, RAA works as the major optimizer of PSOpS. The name of RAA method reflects the steps it follows to optimize the pumping schedule: it first ranks the concentration gradients and then assigns the pumping demand to the water-supply wells according to their ranks and capacities. The detailed procedure is illustrated in Figure 4.2. In the figure, $C_i^{(k)}$ is the contaminant concentration of stress period $i$ after the $k^{th}$ iteration (ML$^{-3}$); $(\partial C_i/\partial q_{ij})^{(k)}$ is the change of contaminant concentration caused by a unit change of $q_{ij}$ after the $k^{th}$ iteration; $SQ_i^{(k)}$ is the sequence of $(\partial C_i/\partial q_{ij})^{(k)}$; and $q_i^{(k)}$ is the pumping rate vector for stress period $i$ after the $k^{th}$ iteration (L$^{3}$T$^{-1}$).

Following the procedure given in Figure 4.2, RAA method optimizes the pumping schedules by first calculating the concentration gradients with respect to pumping rates at the starting point (initial pumping schedule). The gradients are then ranked to form a sequence, and the pumping schedule is updated by assigning the total pumping demand to the pumping wells according to their ranks. For a maximization problem, pumping well with the largest gradient ranks highest and is first assigned a pumping rate. If the total demand is less than its capacity, the total demand is assigned to the well, or otherwise the capacity of the well is assigned as its pumping rate. The remaining pumping demand is assigned to the next well in the sequence in the same manner. This process continues until all pumping demand is assigned to wells.
Under the updated pumping schedule, the concentration gradients are calculated and ranked again. The new rank sequence is then compared to the old one. If these two sequences are same, the RAA method has converged. Otherwise the pumping schedule will be updated again according to the new sequence, and contaminant concentrations under the two updated pumping schedules are compared. For a maximization case, if the concentration under the newly updated schedule is higher, the schedule will be updated using RAA method again. Otherwise the schedule will need to be updated by the IG method.

RAA method typically converges within two iterations, and the total number of objective function evaluations would be $2(n+1)$, with $n$ being the number of candidate
wells. This number is much less than those of regular nonlinear optimization methods and requires less computational demand. Once the RAA method converges, the updated pumping schedule that satisfies the condition \( SQ_i^{(0)} = SQ_i^{(1)} \) is at least a local optimum because it satisfies the Kuhn-Tucker conditions [Kuhn and Tucker, 1951]. The proof of this conclusion is given in Appendix A. The Kuhn-Tucker conditions are the necessary conditions for a solution to be optimum. For an optimization problem with convex objective function, the Kuhn-Tucker conditions are also sufficient conditions for the solution to be a global optimum. However, for a complex contaminant transport problem, the objective function in Equation (4.1) is usually nonconvex. Therefore, the solution obtained by using a RAA method is not guaranteed to be the global optimum, which is a common drawback for gradient-based nonlinear programming methods. In this sense, the RAA method trades computational efficiency with global optimality. The results can be improved by using various starting points if necessary.

### 4.2.2 Improved Gradient Method

As indicated in Figure 4.1, the RAA method is applied first to each stress period. The IG method is only applied in case the RAA method fails to converge. The IG method is similar to the steepest descent method [Press et al., 1989] but includes improvements for the following purposes: (i) reducing the number of dimensions of the optimization problem for computational efficiency; and, (ii) projecting gradients to satisfy the equality constraints.
The IG method works through the steps shown in Figure 4.3, in which $d^{(k)}$ is the search direction of the optimal solution for the $k^{th}$ iteration; $\lambda_k$ is the step size of the solution increment for the $k^{th}$ iteration; $\nabla C_i(q_i^{(k)})$ is the projection of $\nabla C_i(q_i^{(k)})$ in the feasible solution space, with $\nabla C_i(q_i^{(k)})$ being the concentration gradient vector; and $\varepsilon$ is the pre-defined termination criterion.

In the IG algorithm, the last two concentration gradient sequences from the RAA method are first compared to eliminate pumping wells with same ranks in both sequences. The concentration gradients for the remaining pumping wells are then projected to the feasible solution space by subtracting the same amount from all the derivatives to make the summation of the resulting derivatives to be zero. The equality
constraint of the optimization problem can be eliminated by applying this gradient projection because the process guarantees the summation of the resulting pumping rates to be constant.

By following the search direction (the projected gradient vector), the step size maximizing $C_i(q_i^{(k)} + \lambda d^{(k)})$ is obtained by using the one-dimensional line search method, which is then used to update the pumping schedule. If the stopping criterion is met (i.e., the distance between $q_i^{(k)}$ and $q_i^{(k+1)}$ is less than $\varepsilon$), the IG method has converged; otherwise the process is repeated again.

As can be seen from the explanations above, by using RAA and IG methods as optimizers, the computational efficiency of PSOPs is improved significantly.

4.3 Application of PSOPs to a Simple Case

To test the efficiency and reliability of PSOPs, an example problem is created. In the example problem, applications of PSOPs to three different pumping well distributions associated with a hypothetical contaminated site are tested. As shown in Figure 4.4, the unconfined homogeneous aquifer is bounded by no-flow boundaries to its North and South. The east and west boundaries are constant head boundaries with heads of 36 feet and 40 feet, respectively. The dimensions of the site are 2,700 feet × 1,990 feet × 50 feet, which is simulated using 270 columns, 199 rows, and 1 layer in MODFLOW and MT3DMS. Each node has the same dimensions of 10 feet × 10 feet × 50 feet. The initial groundwater flow in the aquifer is at steady-state. The contaminant plume is formed by releasing a contaminant at the node located at row 100 and column 70 at a constant rate of 500 g/day for 10 years, which yields a symmetric plume along the center line of the
site. Other properties of the site and the contaminant used in this example are given in Table 4.1.

![Figure 4.4. Initial contaminant concentration and pumping well distributions for the example problem (concentration unit: ppb)](image)

Table 4.1. Values of parameters used in the example problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquifer thickness</td>
<td>50 ft</td>
</tr>
<tr>
<td>Aquifer specific yield</td>
<td>0.05</td>
</tr>
<tr>
<td>Hydraulic conductivity</td>
<td>30 ft/day</td>
</tr>
<tr>
<td>Effective porosity</td>
<td>0.2</td>
</tr>
<tr>
<td>Longitudinal dispersivity</td>
<td>25 ft</td>
</tr>
<tr>
<td>Horizontal transverse dispersivity</td>
<td>2.5 ft</td>
</tr>
<tr>
<td>Vertical transverse dispersivity</td>
<td>0.25 ft</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>8.5×10^{-4} ft/day</td>
</tr>
<tr>
<td>Soil bulk density</td>
<td>7.7112×10^{4} g/ft³</td>
</tr>
<tr>
<td>Distribution coefficient</td>
<td>5.0×10^{-6} ft³/g</td>
</tr>
<tr>
<td>Maximum contaminant level</td>
<td>15 ppb</td>
</tr>
<tr>
<td>Contaminant first order reaction rate</td>
<td>5.0×10^{-4} l/day</td>
</tr>
</tbody>
</table>
For the example problem, a stress period is equal to one month in simulation time, and the total pumping demand for each stress period is 3,000 ft³/day. To satisfy the total water supply, three candidate wells with capacities 2,000 ft³/day in each well are provided. For each case, the original pumping rate in each well is 1,000 ft³/day. As indicated in Figure 4.4, the distribution of the first well set (Case I) is symmetric about the plume center line. The distributions of pumping wells for the other two sets (Case II and Case III) are asymmetric. For cases II and III, the locations of wells A and B remain unaltered, while well C is relocated at (110, 140) and (70, 140), respectively. By placing pumping wells in these cases, the resulting pumping schedules from PSOpS can be easily compared to empirical solutions for both symmetric and asymmetric cases so that the efficiency and reliability of PSOpS can be demonstrated. The pumping schedule is then optimized to obtain the earliest and latest arrival time in order for the contaminant concentration in the delivered water to reach 15 ppb.

The optimization results obtained by PSOpS are given in Table 4.2. According to the PSOpS output, the optimum pumping schedules are constant for all the stress periods for all three cases. In Case I, to obtain the earliest arrival time, well A operates at its full capacity, while the remaining pumping demand is evenly shared by wells B and C. The result is quite intuitive because, according to the symmetric distribution of pumping wells and contaminant plume, well A will extract the most contaminant from the aquifer given that the pumping rates for all wells are equal. Sharing of the remaining pumping demand allows the plume center to travel along the center line of the site, which leads to the more contaminant extraction from well A. For the latest arrival problem, all of the pumping demand is evenly distributed to wells B and C for the same reason.
Table 4.2. PSOpS results summary for the example problem

<table>
<thead>
<tr>
<th>Case</th>
<th>Objective</th>
<th>Arrival Time (SP)</th>
<th>Pumping Rates (ft³/day)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Well A</td>
<td>Well B</td>
<td>Well C</td>
<td></td>
</tr>
<tr>
<td>Case I</td>
<td>Original</td>
<td>13</td>
<td>1,000</td>
<td>1,000</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Earliest</td>
<td>7</td>
<td>2,000</td>
<td>500</td>
<td>500</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Latest</td>
<td>47</td>
<td>0</td>
<td>1,500</td>
<td>1,500</td>
<td></td>
</tr>
<tr>
<td>Case II</td>
<td>Original</td>
<td>12</td>
<td>1,000</td>
<td>1,000</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Earliest</td>
<td>6</td>
<td>2,000</td>
<td>0</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Latest</td>
<td>29</td>
<td>0</td>
<td>2,000</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td>Case III</td>
<td>Original</td>
<td>17</td>
<td>1,000</td>
<td>1,000</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Earliest</td>
<td>7</td>
<td>2,000</td>
<td>1,000</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Latest</td>
<td>25</td>
<td>0</td>
<td>1,000</td>
<td>2,000</td>
<td></td>
</tr>
</tbody>
</table>

For the earliest arrival times in the other two cases, well A pumps at its capacity due to its location. The remaining pumping demand is supplied by well C for Case II and by well B for Case III. This demand allocation results from the closeness of well C to the center line relative to the proximity of well B to the center line for Case II, and vice versa for Case III. Thus, a pumping well closer to the plume center line can apparently extract more contaminant given equal pumping rates. For the latest arrival problems, the pumping demand is assigned to the three wells in a reverse manner as indicated in Table 4.2.

Results in Table 4.2 also indicate that significant changes in contaminant arrival time can be caused by pumping schedules variations. If well A were to be inoperative, contaminant arrival time may be delayed significantly. Besides the reasonable results discussed for all the example cases, numerical results of PSOpS indicate that all the pumping schedules are updated by RAA method within two iterations, demonstrating the efficiency of PSOpS.
4.4 Application of PSOpS to Camp Lejeune Model

To evaluate the extreme changes of PCE MCL arrival time at the Tarawa Terrace WTP, PSOpS was applied to the Camp Lejeune model for three times: the first run was to obtain the “earliest” PCE MCL arrival time at the Tarawa Terrace WTP; the second run was to obtain the “latest” arrival time at the WTP; and the third run was to obtain the “latest” arrival time with a restriction that the assigned pumping rate in well TT-26 was not to be less than 25% of its pumping capacity. For concise descriptions of the numerical results, the optimal pumping schedules obtained from the three PSOpS runs are identified as “Maximum Schedule” (Max. Sche.), “Minimum Schedule I” (Min. Sche. I), and “Minimum Schedule II” (Min. Sche. II), respectively. The original pumping schedule used in the calibrated Camp Lejeune model is identified as “Original Schedule” (Org. Sche). In the following sections, simulation results for these three optimal pumping schedules are discussed.

4.4.1 Optimization and Simulation Results for the Maximum Schedule

In the Maximum Schedule obtained from PSOpS, pumping rates are updated for 419 stress periods. Among them, pumping rates from 417 stress periods are updated by the RAA method, which reduces the computational time significantly.

According to the ATSDR’s Camp Lejeune model, as previously discussed, water-supply wells started to pump during January 1952, while ABC One-Hour Cleaners started operations during January 1953. The output of PSOpS indicates that the first 3 months of pumping operation during 1952 had a negligible effect on the PCE concentration at the WTP after ABC One-Hour Cleaners started to release PCE into the groundwater system. Except for those three stress periods, well TT-26 always pumped at its maximum
pumping rate (pumping capacity) in the Maximum Schedule solution, which can be seen from Figure 4.5. This fact may be caused by the proximity of the location of well TT-26 to the ABC One-Hour Cleaners and its locating in the downstream groundwater flow direction relative to the contaminant source. The higher pumping rate in well TT-26 would generate a higher hydraulic gradient between the contaminant source and well TT-26, which results in faster movement of contaminant from the source to well TT-26 and, thus, an earlier contaminant MCL arrival time at the pumping well and the WTP.

Figure 4.5. Pumping rate and pumping capacity of well TT-26 under the Maximum Schedule
4.4.1.1 PCE Distribution in the Groundwater System

While keeping the other input data unchanged, and using the Maximum Schedule as input for the WEL package, MODFLOW and MT3DMS were used to simulate the groundwater flow and PCE transport under the Maximum Schedule.

As expected, a variation in the pumping schedule changes the groundwater flow in the subsurface system. Thus, the PCE fate-and-transport in the aquifer domain also is changed. To illustrate this change, a comparison of the PCE distribution – for stress periods 100, 200, 300, and 400 – in the groundwater system at Tarawa Terrace and vicinity under the Original Schedule and the Maximum Schedule are shown in Figures 4.6 – 4.8 for aquifer layers 1, 3, and 5, respectively. The text at the bottom left corner of each illustration in these figures indicates the pumping schedule, the stress period, and the layer number. For example, “Org_SP100_L1” identifies a plot for PCE distribution in layer 1 at stress period 100 under the Original Schedule.
Figure 4.6. Comparison of PCE distribution in Layer 1 under the Original Schedule and the Maximum Schedule (units: ppb)
Figure 4.7. Comparison of PCE distribution in Layer 3 under the Original Schedule and the Maximum Schedule (units: ppb)
Figure 4.8. Comparison of PCE distribution in Layer 5 under the Original Schedule and the Maximum Schedule (units: ppb)
The results shown in Figures 4.6 – 4.8 indicate that, when compared to the Original Schedule, the PCE contaminant plume under the Maximum Schedule is aggregated into a smaller domain and the front of the plume is directed more toward the location of well TT-26. This is because, under the Maximum Schedule, the higher pumping rate in well TT-26 creates a higher piezometric head gradient towards the location of well TT-26, which causes a faster groundwater flow toward and more contaminant mass entering into well TT-26. Therefore, a higher PCE concentration at well TT-26 is expected under the Maximum Schedule.

4.4.1.2 PCE Concentration at Water-Supply Wells

From the concentration observation file obtained from the MT3DMS simulation, the PCE concentrations in water-supply wells are acquired. The results are compared to the PCE concentration distribution under the Original Schedule as shown in Figure 4.9.
Figure 4.9. PCE concentrations at water-supply wells under the Original Schedule and the Maximum Schedule

The results presented in Figure 4.9 lead to the following observations for PCE concentrations at the water-supply wells under the Maximum Schedule:

i. Instead of nine water-supply wells (well TT-23, TT-25, TT-26, TT-31A, TT-31B, TT-53, TT-54A, TT-54B, and TT67) that had PCE concentrations greater than 0.001 ppb under the Original Schedule, under the Maximum Schedule there are only five pumping wells (TT-23, TT-25, TT-26, TT-54A, and TT-54B) that had PCE concentrations higher than 0.001 ppb;

ii. Throughout the simulation period, PCE concentrations at well TT-26 are always higher under the Maximum Schedule when compared to the concentrations obtained under the Original Schedule. More specifically, PCE concentrations at
well TT-26 are much higher under the Maximum Schedule when compared with the Original Schedule results during POI (1968 – 1985);

iii. PCE concentration at well TT-25 is higher under the Maximum Schedule when compared with the Original Schedule results before October 1985 and is lower after that;

iv. For wells TT-23, TT-54A, and TT-54B, the PCE concentrations are lower under the Maximum Schedule when compared with the concentrations obtained under the Original Schedule;

v. Under the Maximum Schedule, only three water-supply wells (TT-23, TT-25, and TT-26) have PCE concentrations over 5 ppb. Among them, PCE concentration at well TT-26 is much greater than the MCL throughout the period of interest. The other two wells have PCE concentrations greater than the MCL only for a very short period of time; and

vi. PCE concentration at well TT-26 is much greater than those obtained in other wells throughout the simulation period. Since well TT-26 always pumped at its full capacity (except for the first three months of 1952), it was the major water-supply well that transported contaminants into the WTP under the Maximum Schedule.

Based on the observations listed above, the difference of the PCE concentrations obtained at well TT-26 using different pumping schedules is further evaluated, and the following observations can be made:

i. PCE concentration at well TT-26 reached 5 ppb during May 1956 under the Maximum Schedule, which is eight months earlier than the PCE MCL arrival
time under the Original Schedule (January 1957). Since well TT-26 was the major contributor of PCE into the WTP, PCE concentration at the WTP also would reach the MCL earlier under the Maximum Schedule;

ii. PCE concentration at well TT-26 is much higher under the Maximum Schedule when compared to the concentration obtained under the Original Schedule during POI. Between these two pumping schedules, the minimum difference of PCE concentration at well TT-26 is 169.62 ppb, the maximum difference is 304.84 ppb, and the average difference is 247.13 ppb (Table 4.3).

<table>
<thead>
<tr>
<th></th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Org. Sche.</td>
<td>312.62</td>
<td>851.19</td>
<td>494.36</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>585.98</td>
<td>1,023.31</td>
<td>741.49</td>
</tr>
<tr>
<td>Difference</td>
<td>304.84</td>
<td>169.62</td>
<td>247.13</td>
</tr>
</tbody>
</table>


4.4.1.3 PCE Concentration at the WTP

Using the volumetric mixing model described in Equation (3.1), PCE concentration at the WTP under the Maximum Schedule was calculated and compared to that obtained under the Original Schedule. These comparisons are shown in Figures 4.10.
Results shown in Figure 4.10 lead to the following observations:

i. The PCE concentration at the WTP under the Maximum Schedule is significantly higher than that obtained from the Original Schedule, except for the time period after February 1985, when well TT-26 was out of service. The higher PCE concentration at the WTP is caused by the higher pumping rate and the higher PCE concentration at well TT-26 under the Maximum Schedule;

ii. The higher PCE concentration at the WTP is equivalent to the earlier contaminant arrival time – the PCE concentration in the Tarawa Terrace WTP reached 5 ppb during December 1956, which is 11 months earlier than the Original Schedule
iii. There are three sudden drops in PCE concentration at the WTP under the Maximum Schedule: July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985. This is similar to what is observed under the Original Schedule and also is caused by well TT-26 being out of service during these periods.

Results shown in Figure 4.10 also indicate that after well TT-26 was shut down during February 1985, PCE concentration at the WTP is lower than that obtained under the Original Schedule, although the absolute difference is small (less than 4 ppb). This phenomenon is caused by the presence of lower PCE concentrations in other water-supply wells. Ten pumping wells (well TT-23, TT-25, TT-31A, TT-31B, TT-52A, TT-52B, TT-54A, TT-54B, TT-67A, and TT-67B) are still in service after February 1985 under the Maximum Schedule. Results shown in Figure 4.9 indicate that, besides water-supply wells with PCE concentrations lower than 0.001 ppb and not shown in the figure, PCE concentrations in all remaining wells are lower under the Maximum Schedule when compared with the results obtained under the Original Schedule during this period.

Lower PCE concentrations in these pumping wells may be attributed to the following:

i. According to results given in Figures 4.6 – 4.8, the higher pumping rate in well TT-26 under the Maximum Schedule causes the PCE plume to aggregate into a smaller region, which in turn causes lower PCE concentrations in the water-supply wells other than TT-26;

ii. More contaminant mass is withdrawn and less mass is left in the groundwater
system under the Maximum Schedule. According to the Camp Lejeune model, $1.40 \times 10^7$ grams of PCE was released into the groundwater system from January 1953 to December 1984. By the time all the pumping operations were terminated (February 1987), $2.45 \times 10^6$ grams of PCE was discharged through the water-supply wells under the Original Schedule, while $4.59 \times 10^6$ grams of PCE was discharged under the Maximum Schedule as indicated in Table 4.4.

### Table 4.4. PCE masses withdrawn under the Original Schedule and the Maximum Schedule

<table>
<thead>
<tr>
<th></th>
<th>Total Mass Released (g)</th>
<th>Mass Withdrawn (g)</th>
<th>Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>$1.40 \times 10^7$</td>
<td>$2.45 \times 10^6$</td>
<td>17.50</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>$1.40 \times 10^7$</td>
<td>$4.59 \times 10^6$</td>
<td>32.78</td>
</tr>
</tbody>
</table>

As discussed previously, there were 15 months during POI when well TT-26 was out of service and the PCE concentration at the WTP was less than 5 ppb. In the other 201 months, PCE concentration at the WTP was greater than the MCL under both the Original Schedule and the Maximum Schedule. A comparison of PCE concentrations at the WTP during those 201 months is summarized in Table 4.5.

### Table 4.5. PCE concentrations at the WTP under the Original Schedule and the Maximum Schedule during POI* (Units: ppb)

<table>
<thead>
<tr>
<th></th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>183.04</td>
<td>46.69</td>
<td>86.39</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>304.66</td>
<td>108.76</td>
<td>166.07</td>
</tr>
<tr>
<td>Difference</td>
<td>180.75</td>
<td>42.67</td>
<td>79.68</td>
</tr>
</tbody>
</table>

4.4.2 Optimization and Simulation Results for Minimum Schedule I

Similar to the Maximum Schedule, PSOpS was run to obtain Minimum Schedule I for the “latest” PCE MCL arrival time at Tarawa Terrace WTP. The results obtained under Minimum Schedule I indicate that well TT-26 pumped at the lowest possible rate for most of the time period (Figure 4.11), which implies that well TT-26 was not put into operation unless there was no other water-supply well available to provide the required total water supply. The reason for this is evident because PCE concentration at well TT-26 is significantly higher than PCE concentration in other pumping wells. For most of the simulation period, lower PCE concentration at the WTP can be realized by reducing the pumping rate of well TT-26. However, there are exceptions to this during the period of late 1970s and early 1980s, which will be discussed in the following section.
4.4.2.1 PCE Distribution in the Groundwater System

Similar to the Maximum Schedule results presented in Figures 4.6 – 4.8, PCE distributions in the subsurface system around Tarawa Terrace and vicinity under the Original Schedule and Minimum Schedule I are compared in Figures 4.12 – 4.14. The notation used in these figures is the same as used for Figures 4.6 – 4.8.

Results presented in Figures 4.12 – 4.14 indicate that Minimum Schedule I also causes a change of PCE distribution in the groundwater system. Opposite to what has been observed under the Maximum Schedule, the contaminant plume under Minimum Schedule I is dispersed to a larger area, and the front of the plume is more away from
well TT-26. Therefore, PCE concentrations at some wells other than well TT-26 are expected to be higher, and PCE concentration at TT-26 is expected to be lower.

According to the results presented in these figures, PCE concentration near well TT-26 is still relatively high due to its closeness to the contaminant source, which causes a greater PCE concentration at well TT-26 when compared to other wells. Therefore, as discussed in previous sections, well TT-26 was pumped at the lowest possible rates for most of the time under Minimum Schedule I to lower the PCE concentration at the WTP.
Figure 4.12. Comparison of PCE distribution in Layer 1 under the Original Schedule and Minimum Schedule I (units: ppb)
Figure 4.13. Comparison of PCE distribution in Layer 3 under the Original Schedule and Minimum Schedule I (units: ppb)
Figure 4.14. Comparison of PCE distribution in Layer 5 under the Original Schedule and Minimum Schedule I (units: ppb)
4.4.2.2 PCE Concentration at Water-Supply Wells

The results of the MT3DMS simulation under Minimum Schedule I provide PCE concentrations at water-supply wells. These results show higher PCE concentrations in some of the pumping wells other than TT-26 (Figure 4.15). Due to the large number of pumping wells with PCE concentrations higher than 0.001 ppb, only wells with PCE concentrations exceeding 5 ppb are shown in Figure 4.15.

![Figure 4.15. PCE concentrations at water-supply wells under the Original Schedule and Minimum Schedule I](image)

From the results shown in Figure 4.15, the following may be observed:

i. Instead of six water-supply wells (TT-23, TT-25, TT-26, TT-54A, TT-54B, and
TT-67) having PCE concentrations exceeding 5 ppb, as seen with the Original Schedule, nine pumping wells have PCE concentrations exceeding 5 ppb under Minimum Schedule I. These wells are TT-23, TT-25, TT-26, TT-31A, TT-31B, TT-54A, TT-54B, TT-67A, and TT-67B. As discussed in the previous sections, this is caused by the generation of a more dispersed contaminant plume under Minimum Schedule I;

ii. PCE concentration at well TT-26 is always less under Minimum Schedule I than under the Original Schedule throughout the simulation period;

iii. Well TT-26 is the first well to have a PCE concentration exceeding PCE MCL. During the first half of the simulation period, well TT-26 is the only well with a PCE concentration greater than 5 ppb. Therefore, well TT-26 is still critical to the PCE MCL arrival time at the WTP;

iv. PCE concentration at well TT-26 exceeds 5 ppb during August 1959 under Minimum Schedule I, which is 31 months later than the case for the Original Schedule (January 1957). This delay would cause a “late” PCE MCL arrival time at the WTP as well; and

v. PCE concentration at well TT-26 is no longer dominant during the second half of the simulation period under Minimum Schedule I. PCE concentrations at wells TT-23, TT-67A, and TT-67B are sometimes greater than that at well TT-26. Higher PCE concentrations at these pumping wells also explain why well TT-26 is not always pumping at the lowest possible rates toward the end of the simulation period – with several pumping wells having high PCE concentrations, Minimum Schedule I is managed in such a way that the plume front is not led to
any particular water-supply well.

4.4.2.3 PCE Concentration at the WTP

The PCE concentration at Tarawa Terrace WTP under Minimum Schedule I is calculated using Equation (3.1) and is shown in Figure 4.16.

Figure 4.16. PCE concentrations at the WTP under the Original Schedule and Minimum Schedule I

The results shown in Figure 4.16 lead to the following observations:

i. PCE concentration at the WTP under Minimum Schedule I is lower than that obtained under the Original Schedule except for the period after February 1985;

ii. PCE concentration at the WTP reaches 5 ppb during June 1960 under Minimum
Schedule I, which is 31 months later than the arrival time of the Original Schedule. This is due to lower PCE concentration and lower pumping rate in well TT-26 under Minimum Schedule I. According to Figure 4.15, by the time the PCE concentration at the WTP reaches 5 ppb, the PCE concentrations at supply wells other than TT-26 are still negligible. Therefore, well TT-26 is the critical well affecting the PCE MCL arrival time at the WTP;

iii. Under Minimum Schedule I, PCE concentration at the WTP increases steadily until December 1961, when PCE concentration dropped below trace levels because of no pumping in well TT-26. PCE concentration reached 5 ppb again during November 1977. Between January 1962 and December 1971, PCE concentration at the WTP is less than 0.001 ppb and, therefore, is not shown in these figures; and

iv. The sudden PCE concentration declines that were observed during periods of July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 under the Original Schedule are not obvious under the Minimum Schedule I for two reasons. First, overall PCE concentration level at the WTP is very low under Minimum Schedule I. Second, PCE concentration at well TT-26 is no longer dominant as shown in Figure 4.15.

Another observation that can be made from the results presented in Figure 4.16 is that during the last 11 months of the POI, PCE concentrations at the WTP under Minimum Schedule I are slightly higher than those obtained under the Original Schedule, which is in contrast to the results obtained under the Maximum Schedule. The reason for this is the higher PCE concentrations in some water-supply wells other than well TT-26
(i.e., well TT-67A and TT-67B). The higher PCE concentrations in these pumping wells may be caused by the following factors:

i. As shown in Table 4.6, by the end of POI, less contaminant mass is extracted from the groundwater system under Minimum Schedule I, and more mass is left in the aquifer, which causes higher PCE concentrations at water-supply wells;

ii. Minimum Schedule I causes a more dispersed contaminant plume in the groundwater system than the Original Schedule. While PCE concentration at well TT-26 decreases, the PCE concentrations at some other wells increase.

<table>
<thead>
<tr>
<th>Total Mass Released (g)</th>
<th>Mass Withdrawn (g)</th>
<th>Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>1.40×10⁷</td>
<td>2.45×10⁶</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>1.40×10⁷</td>
<td>1.98×10⁶</td>
</tr>
</tbody>
</table>

Minimum Schedule I yields lower PCE concentrations at the WTP during POI (Table 4.7). To keep this comparison consistent with the previous comparison made for the Maximum Schedule, the concentration distribution obtained from the 15 months when well TT-26 was out of service is not included in this analysis. The results shown in Table 4.7 indicate that the average PCE concentration at the WTP under Minimum Schedule I is 5.01 ppb, which is close to the 5 ppb MCL of PCE.
Table 4.7. PCE concentrations at the WTP under the Original Schedule and Minimum Schedule I during POI* (Units: ppb)

<table>
<thead>
<tr>
<th></th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>183.04</td>
<td>46.69</td>
<td>86.39</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>41.36</td>
<td>7.84×10^{-8}</td>
<td>5.01</td>
</tr>
<tr>
<td>Difference</td>
<td>158.48</td>
<td>46.69</td>
<td>81.39</td>
</tr>
</tbody>
</table>


4.4.3 Optimization and Simulation Results for Minimum Schedule II

Results obtained under Minimum Schedule I indicate that well TT-26 was out of service for a long period of time, which is unrealistic based on the historical records and considering that well TT-26 was one of the major water-supply wells in the Tarawa Terrace area. Therefore, a third PSOpS simulation was conducted to obtain a pumping schedule that could yield the “latest” arrival time but at the same time honor historical data on the schedule of operations at the site. To achieve this, one more constraint was added to the optimization model – the pumping rate in well TT-26 is restricted to never being less than 25% of its pumping capacity at any time when in service. The pumping rate of well TT-26 obtained for this case is shown in Figure 4.17. Similar to Minimum Schedule I, the pumping rate for well TT-26 for Minimum Schedule II also is the minimum possible during the first half of the simulation period.
4.4.3.1 PCE Distribution in the Groundwater System

PCE distribution in the subsurface system at Tarawa Terrace and vicinity under the Original Schedule and Minimum Schedule II are shown in Figures 4.18 – 4.20 for different stress periods for model layers 1, 3, and 5, respectively. Comparisons of PCE distributions obtained under Minimum Schedules I and Minimum Schedule II are shown in Figures 4.21 – 4.23. The notations used in these figures are same as used in Figure 4.6.

A comparison of Figures 4.12 – 4.14 and Figures 4.18 – 4.23 indicated that Minimum Schedule II also causes the PCE plume to be more dispersed than the Original Schedule, but not as much as Minimum Schedule I. This is because the average pumping
rate in well TT-26 under Minimum Schedule II is less than that obtained under the Original Schedule, but greater than the average pumping rate obtained under Minimum Schedule I. Therefore, PCE concentrations at well TT-26 and the WTP under Minimum Schedule II are expected to be between those obtained under the Original Schedule and Minimum Schedule I.
Figure 4.18. Comparison of PCE distribution in Layer 1 under the Original Schedule and Minimum Schedule II (units: ppb)
Figure 4.19. Comparison of PCE distribution in Layer 3 under the Original Schedule and Minimum Schedule II (units: ppb)
Figure 4.20. Comparison of PCE distribution in Layer 5 under the Original Schedule and Minimum Schedule II (units: ppb)
Figure 4.21. Comparison of PCE distribution in Layer 1 under Minimum Schedule I and Minimum Schedule II (units: ppb)
Figure 4.22. Comparison of PCE distribution in Layer 3 under Minimum Schedule I and Minimum Schedule II (units: ppb)
Figure 4.23. Comparison of PCE distribution in Layer 5 under Minimum Schedule I and Minimum Schedule II (units: ppb)
4.4.3.2 PCE Concentration at Water-Supply Wells

Similar to results presented in Figure 4.15, PCE concentrations at water-supply wells which have PCE concentrations exceeding 5 ppb are plotted in Figure 4.24 for Minimum Schedule II. A comparison of the PCE concentrations at major water-supply wells during POI is shown in Figure 4.25.

![Figure 4.24. PCE concentrations at water-supply wells under the Original Schedule and Minimum Schedule II](image-url)
Results summarized in Figures 4.24 and 4.25 show that PCE concentration distribution at water-supply wells under Minimum Schedule II is similar to the distribution obtained under Minimum Schedule I. The differences for this case are: (1) PCE concentration at well TT-26 under Minimum Schedule II always exceeds that obtained under Minimum Schedule I for most of the POI, and (2) PCE concentrations at wells TT-54A, TT-54B, TT-67A, and TT-67B are slightly higher than those obtained under Minimum Schedule I (Figure 4.25). This is because, as discussed in the previous section, continuous operation of well TT-26 yields a less dispersed PCE plume in the groundwater system and the contaminant plume is more directed toward well TT-26.
Higher PCE concentrations at well TT-26 cause a relatively early PCE MCL arrival time at this location. According to the simulation results, PCE concentration at well TT-26 reached MCL during March 1959 under Minimum Schedule II, which is five months earlier than that obtained under Minimum Schedule I (August 1959). Thus, an earlier PCE MCL arrival time at the WTP is expected for Minimum Schedule II.

4.4.3.3 PCE Concentration at the WTP

PCE concentration at Tarawa Terrace WTP under Minimum Schedule II is shown in Figure 4.26. To illustrate the difference in PCE concentration between the two minimum schedules, PCE concentration obtained at the WTP under Minimum Schedule I is also shown in this figure.
Figure 4.26. PCE concentrations at the WTP under the Original Schedule, Minimum Schedule I, and Minimum Schedule II

Based on results presented in Figure 4.26, the following observations can be made:

i. PCE concentration at the WTP under Minimum Schedule II is lower than that obtained under the Original Schedule except for the period after February 1985, which is similar to the Minimum Schedule I results;

ii. PCE concentration at the WTP reached 5 ppb during February 1960 under Minimum Schedule II, which is four months earlier than that obtained under Minimum Schedule I and a delay of 27 months when compared to the Original Schedule (November 1957);
Before January 1978, PCE concentration at the WTP under Minimum Schedule II is higher than that obtained under Minimum Schedule I, but the difference is minimal after that time. This is because the pumping rate of well TT-26 under Minimum Schedule II after January 1978 is similar to that of Minimum Schedule I; and

Due to the continuous pumping schedule of well TT-26 under Minimum Schedule II, PCE concentration at the WTP does not decrease below 1 ppb. In fact, PCE concentrations at the WTP are greater than 5 ppb most of the time after exceeding the MCL during February 1960, except for the period March 1970 – September 1977.

The total mass of contaminant withdrawn from the groundwater system by water-supply wells under the three pumping schedules is listed in Table 4.8. PCE concentrations at the WTP for the three pumping schedules are compared in Table 4.9. Based on the results given in Tables 4.8 and 4.9, it can be concluded that by forcing the pumping rate of well TT-26 to be at least 25% of its pumping capacity throughout the simulation period, when compared to Minimum Schedule I, about 72% more PCE mass is withdrawn by pumping wells under Minimum Schedule II. Furthermore, the average PCE concentration at the WTP for the POI is approximately 60% higher.

Table 4.8. PCE masses withdrawn under the Original Schedule, Minimum Schedule I, and Minimum Schedule II

<table>
<thead>
<tr>
<th></th>
<th>Total Mass Released (g)</th>
<th>Mass Withdrawn (g)</th>
<th>Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>1.40×10^7</td>
<td>2.45×10^6</td>
<td>17.50</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>1.40×10^7</td>
<td>1.98×10^3</td>
<td>1.41</td>
</tr>
<tr>
<td>Min. Sche. II</td>
<td>1.40×10^7</td>
<td>3.41×10^3</td>
<td>2.44</td>
</tr>
</tbody>
</table>
Table 4.9. PCE concentrations at the WTP under the Original Schedule, Minimum Schedule I and Minimum Schedule II during POI* (Units: ppb)

<table>
<thead>
<tr>
<th></th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>183.04</td>
<td>46.69</td>
<td>86.39</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>41.36</td>
<td>7.84×10⁻⁸</td>
<td>5.01</td>
</tr>
<tr>
<td>Min. Sche. II</td>
<td>45.31</td>
<td>3.04</td>
<td>8.04</td>
</tr>
</tbody>
</table>


4.4.4 Summary of Simulation Results

4.4.4.1 Pumping Rate in Well TT-26

Based on results discussed in previous sections, it may be concluded that the pumping schedule variation causes significant changes in contaminant concentrations and MCL arrival times at water-supply wells and the WTP. For the Camp Lejeune model, the pumping rate in well TT-26 is critical to the PCE MCL arrival time because of its proximity to the contaminant source. The change of pumping rate in well TT-26 can cause PCE concentration at the WTP to change from trace levels to amounts several orders higher than the MCL. The pumping rate percentage in well TT-26 relative to its pumping capacity under different pumping schedules is summarized in Figure 4.27.

Based on the results shown in Figure 4.27, the period January 1962 – February 1976 is when the pumping rate in well TT-26 could have varied the most. This period also is consistent with the most variation of PCE concentrations that is observed at water-supply wells and the Tarawa Terrace WTP under different pumping schedules. The periods when well TT-26 is out of service are consistent with the sudden declines of PCE concentration observed at the WTP under the Original Schedule and the Maximum Schedule.
According to results presented in Figure 4.27, except for the first few months when pumping schedule has no significant effect on PCE concentration, well TT-26 is always being operated at its full capacity for early arrival simulations. Under the Maximum Schedule, PCE concentration at well TT-26 is always much higher than other water-supply wells. Therefore, operation of well TT-26 at 100% capacity is required to obtain the maximum PCE concentration and the earliest arrival of PCE at the WTP. Under the two “late” arrival schedules, however, TT-26 is not pumping at the least possible rates for some stress periods near the end of the simulation. This occurs because
in the second half of the simulation period for the “late arrival” cases, PCE concentration at well TT-26 is no longer the dominant source of contaminants.

4.4.4.2 PCE Concentration at Well TT-26

Simulation results for all three updated pumping schedules show that these schedules can cause changes in PCE distribution in the groundwater system, in PCE concentrations at water-supply wells and the WTP, and in PCE MCL arrival times. The comparison of PCE concentrations at water-supply well TT-26 under different pumping schedules is shown in Figure 4.28.

![Figure 4.28. PCE concentrations at well TT-26 under the Original and updated pumping schedules](image-url)
From results shown in Figure 4.28, it can be concluded that the earliest time for PCE concentration at well TT-26 to reach the 5 ppb MCL is May 1956, and the latest date is August 1959. This indicates that given the hydrogeologic data – together with, and only with – a change of pumping schedules, the 5 ppb arrival time of PCE at well TT-26 can vary from May 1956 to August 1959. This shows a 39-month variability between the “earliest” and “latest” arrival dates. In this figure, the difference observed in the PCE MCL arrival time under Minimum Schedule I is larger than the one observed under the Maximum Schedule relative to the Original Schedule results. The reason for this is, as shown in Figure 4.27, the change of pumping rate in well TT-26 during the first half of the simulation period under Minimum Schedule I is greater than the change under the Maximum Schedule. Furthermore, the greater difference yields a more dispersed contaminant plume and a much lower PCE concentration at well TT-26. A summary of PCE concentrations and MCL arrival times at well TT-26 is given in Table 4.10.

Table 4.10. PCE concentrations and MCL arrival times at well TT-26 under the Original and updated pumping schedules during POI* (Units: ppb)

<table>
<thead>
<tr>
<th>Pumping Schedule</th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
<th>Arrival Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Org. Sche.</td>
<td>851.19</td>
<td>312.62</td>
<td>490.62</td>
<td>01/1957</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>1023.32</td>
<td>585.98</td>
<td>738.40</td>
<td>05/1956</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>144.74</td>
<td>24.49</td>
<td>58.28</td>
<td>08/1959</td>
</tr>
<tr>
<td>Min. Sche. II</td>
<td>243.00</td>
<td>44.32</td>
<td>85.49</td>
<td>03/1959</td>
</tr>
</tbody>
</table>

4.4.4.3 PCE Concentration at the WTP

PCE concentrations at the Tarawa Terrace WTP calculated from different pumping schedules are shown in Figure 4.29. Results shown in this figure indicate that PCE concentration at the Tarawa Terrace WTP could reach the 5 ppb MCL as early as December 1956, or as late as June 1960. Compared to the PCE MCL arrival time at the WTP under the Original Schedule (November 1957), PCE concentration at the WTP could reach the MCL 11 months earlier or 31 months later.

Figure 4.29. PCE concentrations at the WTP under the Original and updated pumping schedules
These results are obtained without changing other parameters that could affect the fate-and-transport of PCE in the subsurface and, thus, the 5 ppb PCE MCL arrival time at the WTP. Therefore, the variation of pumping schedule has an important effect on PCE concentration at the Tarawa Terrace WTP and on the MCL arrival time. A summary of the PCE concentration and MCL arrival time at the WTP under different pumping schedules is listed in Table 4.11.

Table 4.11. PCE concentrations and MCL arrival times at the WTP under the Original and updated pumping schedules during POI* (Units: ppb)

<table>
<thead>
<tr>
<th>Pumping Schedule</th>
<th>Maximum</th>
<th>Minimum</th>
<th>Average</th>
<th>Arrival Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Org. Sche.</td>
<td>183.04</td>
<td>46.69</td>
<td>86.39</td>
<td>11/1957</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>304.66</td>
<td>108.76</td>
<td>166.07</td>
<td>12/1956</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>41.36</td>
<td>7.84×10⁻⁸</td>
<td>5.01</td>
<td>06/1960</td>
</tr>
<tr>
<td>Min. Sche. II</td>
<td>45.31</td>
<td>3.04</td>
<td>8.04</td>
<td>02/1960</td>
</tr>
</tbody>
</table>


Variation of pumping schedules also changes the amount of contaminant mass withdrawn from the groundwater system. A summary of PCE masses withdrawn under different schedules is given in Table 4.12, which indicates a significant change of mass withdrawn from the groundwater system.

Table 4.12. PCE masses withdrawn under the Original and updated pumping schedules

<table>
<thead>
<tr>
<th></th>
<th>Total Mass Released (g)</th>
<th>Mass Withdrawn (g)</th>
<th>Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orig. Sche.</td>
<td>1.40×10⁷</td>
<td>2.45×10⁶</td>
<td>17.50</td>
</tr>
<tr>
<td>Max. Sche.</td>
<td>1.40×10⁷</td>
<td>4.59×10⁶</td>
<td>32.78</td>
</tr>
<tr>
<td>Min. Sche. I</td>
<td>1.40×10⁷</td>
<td>1.98×10⁵</td>
<td>1.41</td>
</tr>
<tr>
<td>Min. Sche. II</td>
<td>1.40×10⁷</td>
<td>3.41×10⁵</td>
<td>2.44</td>
</tr>
</tbody>
</table>
4.5 Summary

In this chapter, the simulation/optimization (S/O) procedure PSOpS is proposed for evaluating the extreme changes of contaminant arrival time at an exposure point caused by variations in historically reconstructed pumping schedules. The goal of the development of PSOpS is to improve the computational efficiency, and this has been achieved as follows:

i. *The reduction of the dimension of the optimization problem:* By reformulating the optimization problem, the pumping schedule of only the current stress period instead of the current and all previous stress periods needs to be optimized for the optimum contaminant concentration, which makes the dimension of the problem to a computationally manageable magnitude. Utilization of IG optimization method can reduce the dimension of the problem as well by eliminating pumping wells with equal ranks;

ii. *The reduction of the number of iterations:* As the major optimizer of PSOpS, the RAA method usually converges within two iterations, which means less objective function evaluation and much less computational demand; and,

iii. *Elimination of repeated simulations:* Using the piezometric head and concentration distributions under the optimum pumping schedule of the previous stress period as the initial condition eliminates the need of repeated computationally-expensive groundwater flow and contaminant transport simulations.

The efficiency and reliability of PSOpS were demonstrated using a simple example problem. PSOpS was then applied to Camp Lejeune model to evaluate the effect
of pumping schedule variation on PCE concentration and MCL arrival time at Tarawa Terrace WTP. Simulation results for the Camp Lejeune model lead to the following conclusions:

i. Variation of pumping schedule has an effect on contaminant arrival time at water-supply wells. According to study results, a change in pumping schedules can cause changes in the contaminant plume distribution and the orientation of the plume front in the groundwater system. Changes in the contaminant transport characteristics lead to a variation of contaminant concentrations at water-supply wells, which is equivalent to the variation of contaminant arrival time at the water-supply wells. For example, according to the results presented herein, the arrival time of 5 ppb PCE concentration at well TT-26 varies from May 1956 to August 1959;

ii. Variation of pumping schedules has an impact on the contaminant arrival time at the WTP, and this impact is twofold. The volumetric mixing model equation indicates that PCE concentration at the WTP is calculated using PCE concentrations and pumping rates at water-supply wells. Therefore, a variation of pumping schedule changes the contaminant arrival time at the WTP by affecting both quantities of the volumetric mixing model equation. Simulation results reported in this chapter indicate that the PCE MCL arrival time at the WTP varies from December 1956 to June 1960. This outcome is based on the allowable changes to pumping schedules within the pumping capacity of each well;

iii. Water-supply well TT-26 is critical for assessing the contaminant arrival time at the WTP. All simulation results show that by the time PCE concentration at the
WTP reaches 5 ppb, PCE concentrations at all water-supply wells, except well TT-26, are still negligible. This is due to some unique characteristics of well TT-26. First, well TT-26 is the closest water-supply well to the contaminant source, ABC One-Hour Cleaners. Second, well TT-26 is located in the down-gradient groundwater-flow direction relative to the contaminant source. Third, well TT-26 has the longest pumping history among all water-supply wells. Therefore, increasing the pumping rate in well TT-26 can cause earlier contaminant arrival time at the WTP, and vice versa;

iv. Variation of pumping schedules can cause a significant change in the amount of contaminant mass withdrawn from the groundwater system. Considering the total amount of water supplied to the WTP, a change in PCE concentration at the WTP caused by a variation in the pumping schedules leads to a change in contaminant mass withdrawn. Given different pumping schedules derived in this study, the total PCE mass that was supplied to the WTP could vary from 1.41% to 32.78% of the total contaminant mass released from the contaminant source into the groundwater system at the site.

Based on the optimal pumping schedules obtained from PSOpS, simulations have been conducted to demonstrate the effect of the pumping schedule variation on PCE arrival times at water-supply wells and the Tarawa Terrace WTP. Analyses of simulation results indicate that a variation in pumping schedules can affect the PCE arrival time. Considering this uncertainty factor, a change of pumping schedules yields the following outcomes: (i) PCE MCL arrival time at well TT-26 varies from May 1956 to August
1959, and (ii) PCE MCL arrival time at the Tarawa Terrace WTP varies from December 1956 to June 1960.
CHAPTER 5

UNCERTAINTY ANALYSIS OF CAMP LEJEUNE MODEL

The Agency for Toxic Substances and Disease Registry (ATSDR), U.S. Department of Health and Human Services, is conducting an epidemiologic study at U.S. Marine Corps Base Camp Lejeune, North Carolina, to determine if exposure to contaminated drinking water is related to birth defects and childhood cancer in children born to women who lived on base during the period 1968 – 1985. Due to limited measurements of contaminant and exposure data available for the health study, ATSDR has historically reconstructed the groundwater flow and contaminant fate-and-transport simulations (i.e., Camp Lejeune model) at the site to fill in the data gap.

The nature of a historical reconstruction determines that there are inevitably uncertainties associated with the input data, and therefore, the final results of simulations models, which may seriously impact the reliability of related health studies. According to discussions in the previous two chapters, the critical uncertain variables that take the most uncertainties into the final results of Camp Lejeune model can be identified as follows: hydraulic conductivities in layers 1, 3, and 5; pumping schedule; effective porosity; first order reaction rate; contaminant mass loading rate; recharge rate; soil bulk density; distribution coefficient; and longitudinal dispersivity. In this chapter, the uncertainties residing in the simulation results of Camp Lejeune model caused by these uncertain parameters are evaluated by conducting an uncertainty analysis.

As introduced in the literature review, the application of analytical uncertainty analysis methods toward a real-world problem is prohibitive because of its requirements
such as simple functional relationships and independence of stochastic variables [Tung and Yen, 2005]. The Taylor series expansion methods, such as first and second moment method, are also inapplicable for this study because of the tremendous computational requirement associated with the numerical evaluation of sensitivity coefficients [Tung and Yen, 2005]. Therefore, the uncertainties associated with simulation results of Camp Lejeune model were evaluated by using Monte Carlo simulation (MCS) method. Considering the computational burden caused by the large size and complexity of Camp Lejeune model, a few improvements were made to MCS to achieve computational efficiency. To demonstrate the effect of pumping schedule variation on PCE concentration at the WTP, two MCS processes were conducted: Scenario 1 and Scenario 2. For Scenario 1, the pumping schedule variation is excluded from the uncertainty analysis; in Scenario 2, all the nine critical uncertain variables listed above were included in the analysis.

5.1 Introduction to Monte Carlo Simulation

Monte Carlo simulation (MCS) is a statistical uncertainty analysis tool that has been considered to be the main method in groundwater hydrology for assessing the uncertainties in groundwater flow and contaminant transport predictions caused by input uncertainties [Ballio and Guadagnini, 2004]. MCS evaluates the distribution of system responses subject to input uncertainties by measuring system responses repeatedly under various realizations [Tung and Yen, 2005], wherein a realization is a set of data generated according to their probabilistic distributions as the input for one simulation. A major advantage of MCS is that it can be easily applied for complex models because no details about the simulation models are required for an MCS analysis.
During a Monte Carlo simulation, numerous equally probable realizations are generated according to the probability distributions of input variables. Simulations are then conducted repeatedly by using these realizations as input. The simulation results are collected and analyzed statistically to provide the probability distribution and statistical properties of the output variables of interest. Detailed procedure of the improved Monte Carlo simulation method that was used to assess uncertainties associated with the simulation results of Camp Lejeune model is provided in Figure 5.1. Comparing Figure 5.1 to Figure 3.2, one can tell that, except the embedded filtering process and statistical module, the improved MCS process resembles repetitive calculations of PCE concentration at the WTP using statistically generated input. As key improvements of reliability and efficiency, the filtering process and statistical module applied in the improved MCS are introduced as follows.

![Figure 5.1. Illustration of the improved Monte Carlo simulation](image-url)
5.1.1 Filtering Process

Input data for Monte Carlo simulations are generated according to the probabilistic distribution of uncertain variables. Theoretically, all the realizations are equally probable, and can represent the input parameters equally well. However, sometimes a statistically generated realization may yield simulation results significantly different from the on-site measurements, thus fails to represent the site being studied. Using such realizations in an MCS process may cause misleading conclusions. To make sure that all the simulation results obtained for the uncertainty analysis agree with the on-site measurements, a filtering process is embedded into the improved MCS as indicated in Figure 5.1. It works by checking the simulated piezometric heads at a few monitoring points. If the water head at any monitoring point is out of the feasible range that is pre-defined according to field data, the corresponding realization will be removed from the MCS, thus to avoid taking invalid results to the final statistical analysis.

Particularly, for the Camp Lejeune model case, if any water-supply well dries up or water head in any of the observation points listed in Table 5.1 is out of the valid range (-24 feet to 28 feet) during the MODFLOW simulation, the corresponding simulation will be terminated and replaced by another one. The validity check of a realization prior to further simulations (i.e., MT3DMS simulation and volumetric mixing model) prevents the waste of computational source on invalid realizations.
Table 5.1. Locations of observation points for the filtering process

<table>
<thead>
<tr>
<th>Point</th>
<th>Row</th>
<th>Column</th>
<th>Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12</td>
<td>108</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>78</td>
<td>61</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>83</td>
<td>96</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>74</td>
<td>119</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>111</td>
<td>61</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>120</td>
<td>38</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>111</td>
<td>91</td>
<td>1</td>
</tr>
<tr>
<td>8</td>
<td>134</td>
<td>69</td>
<td>1</td>
</tr>
<tr>
<td>9</td>
<td>166</td>
<td>81</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>141</td>
<td>122</td>
<td>1</td>
</tr>
<tr>
<td>11</td>
<td>137</td>
<td>154</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>132</td>
<td>190</td>
<td>1</td>
</tr>
<tr>
<td>13</td>
<td>112</td>
<td>213</td>
<td>1</td>
</tr>
<tr>
<td>14</td>
<td>97</td>
<td>198</td>
<td>1</td>
</tr>
<tr>
<td>15</td>
<td>75</td>
<td>237</td>
<td>1</td>
</tr>
<tr>
<td>16</td>
<td>46</td>
<td>159</td>
<td>1</td>
</tr>
</tbody>
</table>

5.1.2 Statistical Module

Although the MCS approach has been widely applied as an uncertainty analysis method, it has several disadvantages. A major disadvantage is that it requires a large number of simulation runs [Andricevic, 1993], which means a high computational demand. This is due to the fact that the accuracy of the stochastic properties obtained from MCS is a function of the number of simulation runs – the more realizations included in an MCS, the more accurate would the results be. The high computational cost prevents the application of MCS on complex field-scale simulation models. Another disadvantage of the MCS method is that there is not well-established convergence criterion for an MCS [Ballio and Guadagnini, 2004]. In the improved MCS procedure, an embedded statistical module is applied to check the convergence after each simulation.
Due to the large size of the Camp Lejeune model, the computational demand for the MCS is very intensive. To achieve the computational efficiency, in this study, a stopping criterion is defined so that the Monte Carlo simulation can be terminated as soon as the obtained simulation results are adequate for the uncertainty analysis purpose. The termination criterion is measured by the difference of coefficient of variation (CV), which is defined by the ratio of the standard deviation to the mean of the output variable. After each simulation the mean, variance, and CV for PCE concentration at the WTP in each stress period are evaluated by the statistical module. Once the changes of CVs are less than the predefined threshold, the MCS will be terminated and the results will be analyzed for uncertainty evaluation.

5.2 Generation of Input Data

During an MCS process, simulations are conducted repeatedly by using a large number of equally likely realizations generated according to the probability distributions of input variables. Statistical analysis of the simulation results can then provide the probability distribution and statistical properties of the output variables of interest. As it can be seen, the reliability of an MCS largely depends on the quality of input realizations. Therefore, generation of realizations that can closely preserve the probability distributions of input variables are of great importance. For Camp Lejeune model, there are totally nine different parameters identified as critical uncertain variables. Each of the nine parameters has its own properties and probabilistic distribution. Accordingly, they are generated by using different routines or softwares as introduced below.
5.2.1 Generation of Hydraulic Conductivities

In Camp Lejeune model, the hydraulic conductivities in layers 1, 3, and 5 are heterogeneous. Moreover, spatial correlations exist among hydraulic conductivities of each layer. Variogram is a geostatistics concept that is used to characterize this spatial continuity [Barnes]. The mathematical definition of variogram can be written as

\[ \gamma(h) = \frac{1}{2} E\left\{ [Z(x) - Z(x+h)]^2 \right\}, \]

(5.1)

where \( Z(x) \) is the value of parameter Z at location \( x \); \( h \) is the separation distance that is referred to as “lag”; and, \( E[\ ] \) is the statistical expectation operator. The most typical variogram models for groundwater applications include spherical model and exponential model as indicated in Figure 5.2.

![Illustrations of spherical and exponential variogram models](image)

Figure 5.2. Illustrations of spherical and exponential variogram models

The spherical model is defined as
\[
\gamma(h) = \begin{cases} 
c \cdot \left[ 1.5 \frac{h}{a} - 0.5 \left( \frac{h}{a} \right)^3 \right] & \text{if } h < a, \\
c & \text{if } h \geq a
\end{cases}, \tag{5.2}
\]

in which \( c \) is the scale; \( h \) is the lag distance; and \( a \) is the length.

Similarly, the exponential model is defined as

\[
\gamma(h) = c \cdot \left[ 1 - \exp\left(-\frac{h}{a}\right) \right], \tag{5.3}
\]

the terms used in Equation (5.3) are same as those used in Equation (5.2).

FIELDGEN is a two dimensional stochastic field generator that uses variogram to account for the geostatistics properties associated with the field data. It is one of the utilities included in the groundwater data utilities package, and is initiated from Geostatistical Software Library (GSLIB) developed at Stanford [Deutsch and Journel, 1998]. In FIELDGEN, a stochastic field is generated based on conditioning points using the Gaussian sequential simulation principal [Doherty, 2007].

In this study, FIELDGEN was applied to generate the horizontal hydraulic conductivities. The measured hydraulic conductivity values from the Camp Lejeune site were used as conditioning points. Due to the limited availability of field data – 18 points for layer 1, 22 points for layer 3, and 5 points for layer 5 – 100 additional conditioning points were randomly extracted for each layer from the calibrated hydraulic conductivity fields as used in Camp Lejeune model. As indicated in Figures 5.3 – 5.5, 50 data points were picked up within the rectangular zone defined by nodes located at (40, 60) and (110, 200) (i.e., the area defined by dashed lines), in which all the water-supply wells are located. The remaining 50 data points were selected from the whole model domain. Choosing more conditioning points in this region defined by dash lines assures better
representation of hydraulic conductivities in this area, which are more critical for the groundwater flow and contaminant transport. Comparison of hydraulic conductivities in layer 1 between the calibrated Camp Lejeune model and an FIELDGEN generation is illustrated in Figure 5.6. The figure indicates that realization generated by FIELDGEN preserves the spatial distributions of hydraulic conductivities quite well.

Figure 5.3. Illustration of conditioning points for layer 1
Figure 5.4. Illustration of conditioning points for layer 3

Figure 5.5. Illustration of conditioning points for layer 5
5.2.2 Generation of Pumping Schedules

As discussed in Chapter 4, variation of pumping schedule can cause significant change to the PCE MCL arrival time and PCE concentrations at the WTP. In Camp Lejeune model, groundwater flow and contaminant fate-and-transport are simulated for the period of 1951 – 1994. However, the historical pumpage record of Tarawa Terrace shows that there is no pumpage information available for the time period before 1975, indicating there are potential uncertainties associated with the historically reconstructed pumping schedule. To further demonstrate the uncertainties associated with PCE concentration and MCL arrival time that can be caused by pumping schedule variations, uncertainty analyses with and without pumping schedule uncertainty excluded were conducted as Scenario 1 and Scenario 2, respectively.

Prior to generating pumping schedule realizations, historical pumping demand of each stress period was generated first. Historical records for the total pumping rates at Tarawa Terrace are incomplete. Relatively complete records are only available for years
of 1978, 1980 – 1981, and 1983 – 1984, as summarized in Table 5.2. In the table, “N/A” implies that no historical data are available for that time period. Dividing the monthly averaged pumping demand (i.e., \( Q_{T\text{-monthly}} \)) by the yearly averaged water-supply (i.e., \( Q_{T\text{-yearly}} \)) indicated in Table 5.2, the ratios of \( Q_{T\text{-monthly}}/Q_{T\text{-yearly}} \), which can indicate the variation of monthly water demand, are obtained and listed in Table 5.3.

### Table 5.2. Historical pumping demand at Tarawa Terrace (unit: \( \text{ft}^3/\text{day} \))

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan</td>
<td>119,674</td>
<td>125,086</td>
<td>106,089</td>
<td>111,644</td>
<td>103,463</td>
</tr>
<tr>
<td>Feb</td>
<td>135,982</td>
<td>98,563</td>
<td>95,123</td>
<td>110,156</td>
<td>112,682</td>
</tr>
<tr>
<td>Mar</td>
<td>108,621</td>
<td>112,088</td>
<td>109,729</td>
<td>N/A</td>
<td>108,281</td>
</tr>
<tr>
<td>Apr</td>
<td>119,572</td>
<td>91,796</td>
<td>114,599</td>
<td>118,113</td>
<td>111,943</td>
</tr>
<tr>
<td>May</td>
<td>112,722</td>
<td>96,054</td>
<td>116,780</td>
<td>126,212</td>
<td>121,114</td>
</tr>
<tr>
<td>Jun</td>
<td>131,734</td>
<td>105,847</td>
<td>133,186</td>
<td>141,676</td>
<td>116,413</td>
</tr>
<tr>
<td>Jul</td>
<td>128,454</td>
<td>121,037</td>
<td>128,808</td>
<td>137,481</td>
<td>111,394</td>
</tr>
<tr>
<td>Aug</td>
<td>120,174</td>
<td>108,078</td>
<td>123,805</td>
<td>143,216</td>
<td>124,077</td>
</tr>
<tr>
<td>Sep</td>
<td>119,942</td>
<td>104,973</td>
<td>122,291</td>
<td>126,377</td>
<td>113,008</td>
</tr>
<tr>
<td>Oct</td>
<td>135,070</td>
<td>99,043</td>
<td>N/A</td>
<td>N/A</td>
<td>115,538</td>
</tr>
<tr>
<td>Nov</td>
<td>103,271</td>
<td>94,300</td>
<td>N/A</td>
<td>115,952</td>
<td>113,775</td>
</tr>
<tr>
<td>Dec</td>
<td>103,847</td>
<td>97,400</td>
<td>N/A</td>
<td>147,365</td>
<td>108,211</td>
</tr>
<tr>
<td>Average</td>
<td>119,922</td>
<td>104,522</td>
<td>116,712</td>
<td>127,819</td>
<td>113,325</td>
</tr>
</tbody>
</table>

### Table 5.3. \( Q_{T\text{-monthly}}/Q_{T\text{-yearly}} \) ratios at Tarawa Terrace

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan</td>
<td>0.9979</td>
<td>1.1967</td>
<td>0.9090</td>
<td>0.8734</td>
<td>0.9130</td>
</tr>
<tr>
<td>Feb</td>
<td>1.1339</td>
<td>0.9430</td>
<td>0.8150</td>
<td>0.8618</td>
<td>0.9943</td>
</tr>
<tr>
<td>Mar</td>
<td>0.9058</td>
<td>1.0724</td>
<td>0.9402</td>
<td>N/A</td>
<td>0.9555</td>
</tr>
<tr>
<td>Apr</td>
<td>0.9971</td>
<td>0.8782</td>
<td>0.9819</td>
<td>0.9241</td>
<td>0.9878</td>
</tr>
<tr>
<td>May</td>
<td>0.9400</td>
<td>0.9190</td>
<td>1.0006</td>
<td>0.9874</td>
<td>1.0687</td>
</tr>
<tr>
<td>Jun</td>
<td>1.0985</td>
<td>1.0127</td>
<td>1.1411</td>
<td>1.1084</td>
<td>1.0270</td>
</tr>
<tr>
<td>Jul</td>
<td>1.0711</td>
<td>1.1580</td>
<td>1.0366</td>
<td>1.0756</td>
<td>0.9830</td>
</tr>
<tr>
<td>Aug</td>
<td>1.0021</td>
<td>1.0340</td>
<td>1.0608</td>
<td>1.1204</td>
<td>1.0949</td>
</tr>
<tr>
<td>Sep</td>
<td>1.0002</td>
<td>1.0043</td>
<td>1.0478</td>
<td>0.9887</td>
<td>0.9972</td>
</tr>
<tr>
<td>Oct</td>
<td>1.1263</td>
<td>0.9476</td>
<td>N/A</td>
<td>N/A</td>
<td>1.0195</td>
</tr>
<tr>
<td>Nov</td>
<td>0.8612</td>
<td>0.9022</td>
<td>N/A</td>
<td>0.9072</td>
<td>1.0040</td>
</tr>
<tr>
<td>Dec</td>
<td>0.8660</td>
<td>0.9319</td>
<td>N/A</td>
<td>1.1529</td>
<td>0.9549</td>
</tr>
</tbody>
</table>
Statistical analysis results regarding the $Q_{T\text{-monthly}}/Q_{T\text{-yearly}}$ ratios are shown in Table 5.4 and Figure 5.7. It can be observed from Figure 5.7 that within a period of one year, the pumping demands at Tarawa Terrace in June – October are higher than yearly average while water demands in the remaining months are relatively lower. According to this analysis, the total pumping demand of each stress period was generated for the uncertainty analysis of Scenario 2.

Table 5.4. Statistical results of $Q_{T\text{-monthly}}/Q_{T\text{-yearly}}$ ratios at Tarawa Terrace

<table>
<thead>
<tr>
<th>Month</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan</td>
<td>0.9780</td>
<td>0.1305</td>
<td>0.8735</td>
<td>1.1967</td>
</tr>
<tr>
<td>Feb</td>
<td>0.9496</td>
<td>0.1243</td>
<td>0.8150</td>
<td>1.1339</td>
</tr>
<tr>
<td>Mar</td>
<td>0.9685</td>
<td>0.0723</td>
<td>0.9058</td>
<td>1.0724</td>
</tr>
<tr>
<td>Apr</td>
<td>0.9538</td>
<td>0.0510</td>
<td>0.8782</td>
<td>0.9971</td>
</tr>
<tr>
<td>May</td>
<td>0.9831</td>
<td>0.0584</td>
<td>0.9190</td>
<td>1.0687</td>
</tr>
<tr>
<td>Jun</td>
<td>1.0776</td>
<td>0.0552</td>
<td>1.0127</td>
<td>1.1411</td>
</tr>
<tr>
<td>Jul</td>
<td>1.0783</td>
<td>0.0635</td>
<td>0.9830</td>
<td>1.1580</td>
</tr>
<tr>
<td>Aug</td>
<td>1.0624</td>
<td>0.0471</td>
<td>1.0021</td>
<td>1.1205</td>
</tr>
<tr>
<td>Sep</td>
<td>1.0076</td>
<td>0.0232</td>
<td>0.9887</td>
<td>1.0478</td>
</tr>
<tr>
<td>Oct</td>
<td>1.0311</td>
<td>0.0899</td>
<td>0.9476</td>
<td>1.1263</td>
</tr>
<tr>
<td>Nov</td>
<td>0.9186</td>
<td>0.0605</td>
<td>0.8612</td>
<td>1.0040</td>
</tr>
<tr>
<td>Dec</td>
<td>0.9764</td>
<td>0.1236</td>
<td>0.8660</td>
<td>1.1529</td>
</tr>
</tbody>
</table>
As described previously, pumping records for the year of 1978 and years of 1980 and later are relatively detailed. Therefore, during the MCS process, total pumping demands in these time periods remain the same as historical records. Other than those, for each simulation realization, $Q_{T\text{-monthly}}/Q_{T\text{-yearly}}$ ratio of each month is generated according to the statistical results in Table 5.4 using a normal distributed random number generation function, RNNOF, of the IMSL library. The ratios are then multiplied by yearly averaged pumping demands, which are same as used in the calibrated Camp Lejeune model, to generate monthly averaged pumping demand for each stress period. To assure the validity of the generated pumping demand, the demand of each stress period is compared to the total pumping capacity available for the corresponding stress period. If the total demand
exceeds the total capacity, the demand will be set to be equal to the total capacity. One example of the generated water demand is compared to that of the calibrated model in Figure 5.8. In stead of remaining a constant value as in Camp Lejeune model, the generated pumping demand varies by month, thus better represents a real-world case.

![Figure 5.8. Comparison of generated historical pumping demands to calibrated model](image)

After historical pumping demand is generated for each stress period, it is assigned to all active water-supply wells to create the WEL file for MODFLOW simulation. Previous study has shown that well TT-26 is the critical well that has major effect on PCE MCL arrival time and PCE concentration at the WTP. Therefore, the pumping rate
in well TT-26 is assigned first. The remaining demand is then assigned to other water-supply wells according to their capacities. The detailed procedure is described as follows.

i. The ratio $Q_{TT-26}/QC_{TT-26}$ is generated according to a normal distribution with mean of 0.8 and standard deviation of 0.1 using the RNNOF function, where $Q_{TT-26}$ is pumping rate in well TT-26 and $QC_{TT-26}$ is the pumping capacity. The maximum and minimum ratios are 1.0 and 0.0, respectively. This means that well TT-26 is pumping at about 80% of its capacity in a statistical sense;

ii. $Q_{TT-26}$ is calculated according to the ratio $Q_{TT-26}/QC_{TT-26}$ and the pumping capacity of well TT-26 (i.e., $QC_{TT-26}$); and

iii. The total pumping demand is subtracted by $Q_{TT-26}$, and is then assigned to the remaining active water-supply wells according to their pumping capacities – pumping well with a higher capacity will obtain a higher pumping rate in it, and vice versa.

5.2.3 Generation of Other Uncertain Variables

Except for the horizontal hydraulic conductivities and pumping schedule, all the other uncertain parameters applied in the uncertainty analysis are generated using the RNNOF function of IMSL library by following specific rules and probabilistic distributions as described below.

Effective porosity

i. Effective porosities for different cells in the same realization are normally distributed;

ii. Mean value of effective porosities is 0.2;

iii. Standard deviation of effective porosities is 0.05;
iv. Upper limit of effective porosities is 0.3; and
v. Lower limit of effective porosities is 0.1.

First order reaction rate

i. First order reaction rate is constant in one realization;
ii. Reaction rates in various realizations are normally distributed;
iii. Mean value of reaction rates is 0.0005/day;
iv. Standard deviation of reaction rates is 0.000135/day;
v. Upper limit of reaction rates is 0.00077/day; and
vi. Lower limit of reaction rates is 0.00023/day.

Mass loading rate

i. Mass loading rates in different stress periods for the same realization are normally distributed;
ii. Mean value of mass loading rates is 1,200 g/day;
iii. Standard deviation of mass loading rates is 100 g/day;
iv. Upper limit of mass loading rates is 2,200 g/day; and
v. Lower limit of mass loading rates is 200 g/day.

Recharge rate

i. Recharge rates in the same calendar year for one realization are same;
ii. Recharge rates in different realizations for the same calendar year are normally distributed;
iii. Mean value of recharge rate for each calendar year is same as the calibrated value in Camp Lejeune model;
iv. Standard deviation for all the normal distributions are 0.0005 ft/day;

v. Upper limit of recharge rate is 0.005 ft/day; and

vi. Lower limit of recharge rate is 0.001 ft/day.

**Bulk density**

i. Bulk densities of different cells in the same realization are normally distributed;

ii. Mean value of bulk densities is 77,112 g/ft$^3$;

iii. Standard deviation of bulk densities is 1,100 g/ft$^3$;

iv. Upper limit of bulk densities is 79,004 g/ft$^3$; and

v. Lower limit of bulk densities is 69,943 g/ft$^3$.

**Distribution coefficient**

i. Distribution coefficients of different cells in one realization are normally distributed;

ii. Mean value of distribution coefficients is $5.0000 \times 10^{-6}$ g/ft$^3$;

iii. Standard deviation of distribution coefficients is $1.7657 \times 10^{-6}$ g/ft$^3$;

iv. Upper limit of distribution coefficients is $2.6839 \times 10^{-5}$ g/ft$^3$; and

v. Lower limit of distribution coefficients is $3.5315 \times 10^{-6}$ g/ft$^3$.

**Longitudinal dispersivity**

i. The natural logarithms of longitudinal dispersivities in different cells of one realization are normally distributed;

ii. Mean value of the natural logarithms of longitudinal dispersivities is ln(25);

iii. Standard deviation of the natural logarithms of longitudinal dispersivities is ln(5)/2;
iv. Upper limit of longitudinal dispersivities is 125 ft; and

v. Lower limit of longitudinal dispersivities is 5 ft.

A summary of the statistical properties of the uncertain parameters is listed in Table 5.5.

Table 5.5. Statistical properties of uncertain variables used in uncertainty analysis

<table>
<thead>
<tr>
<th>Variable</th>
<th>Mean</th>
<th>STD</th>
<th>Upper Bound</th>
<th>Lower Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective Porosity</td>
<td>0.2</td>
<td>0.05</td>
<td>0.3</td>
<td>0.1</td>
</tr>
<tr>
<td>Reaction Rate (day(^{-1}))</td>
<td>0.00067</td>
<td>0.000135</td>
<td>0.00094</td>
<td>0.00040</td>
</tr>
<tr>
<td>Mass Loading Rate (g/day)</td>
<td>1,200</td>
<td>100</td>
<td>2,200</td>
<td>200</td>
</tr>
<tr>
<td>Recharge Rate (ft/day)</td>
<td>*</td>
<td>0.0005</td>
<td>0.005</td>
<td>0.001</td>
</tr>
<tr>
<td>Bulk Density (g/ft(^3))</td>
<td>77.112</td>
<td>1.100</td>
<td>79,004</td>
<td>69,943</td>
</tr>
<tr>
<td>Distribution Coefficient (g/ft(^3))</td>
<td>5.00×10(^{-6})</td>
<td>1.7657×10(^{-6})</td>
<td>2.6839×10(^{-5})</td>
<td>3.5315×10(^{-6})</td>
</tr>
<tr>
<td>Longitudinal Dispersivity (ft)</td>
<td>Ln(25)**</td>
<td>Ln(5)/2**</td>
<td>125</td>
<td>5</td>
</tr>
</tbody>
</table>

*Mean value of recharge rate for each stress period is same as the calibrated value in Camp Lejeune model.

**The mean and standard deviation are for the natural logarithms of longitudinal dispersivities.

5.3. Simulation Results and Discussion

5.3.1 MCS Results of Scenario 1

For the uncertainty analysis of Scenario 1, a total number of 840 realizations were generated. Among these realizations, 510 simulations passed the filtering process and were completed. Relative changes of CVs of PCE concentration at the WTP for POI (1968 – 1985) were calculated as the number of realizations used in MCS was increased. The relative change of CV is calculated by using the following equation:

\[ R_i = \frac{CV_{i,new} - CV_{i,old}}{CV_{i,old}} \times 100\% , \]  

(5.4)
where \( R_i \) is the relative change of CV value of stress period \( i \); \( CV_{i,\text{new}} \) is the updated CV value by using more simulation results of stress period \( i \); and \( CV_{i,\text{old}} \) is the CV value of PCE concentrations at the WTP in stress period \( i \), which is obtained prior to the update. The obtained results are plotted in Figure 5.9.

In Figure 5.9, the floating bars indicate the range of relative changes of CVs for PCE concentration at the WTP, and the solid line indicates the average of these relative changes. It can be observed from Figure 5.9 that, as the number of realizations used in the MCS increases to 510, both the range and the average of the relative changes go close to zero (0.062% – 0.477 % for the range of relative change, and 0.358% for the average of
relative change). For our study, the range and average of relative changes of CV falling in between -0.5% – 0.5% indicates the convergence of MCS.

Statistical analysis to the PCE concentrations at the WTP obtained from the MCS process reveals the following results:

i. As shown in Figure 5.10, the mean values of PCE concentrations at the WTP for the POI (1968 – 1985) in Scenario 1 is very close to the results of the calibrated Camp Lejeune model from the ATSDR study;

ii. According to the probabilistic analysis, there is a 95% probability that the PCE concentrations at the WTP are within the range defined by the 95% bounds in Figure 5.10;

iii. The mean value of the PCE MCL arrival time at the WTP for Scenario 1 is February 1958, which is three months later than the calibrated result from the ATSDR study;

iv. The PCE concentration at the WTP would exceed the 5 ppb MCL from October 1957 to August 1958 with a probability of 95%, with the calibrated PCE MCL arrival time falling in between (November 1957); and

v. During January 1985, the PCE concentration at the WTP would vary between 110 – 251 ppb with a probability of 95%. This range includes the calibrated value of 176 ppb from Camp Lejeune model, and also the maximum filed-measured value of 215 ppb, which provides a sense of confidence in the historically reconstructed PCE concentrations at the WTP [Suarez-Soto et al., 2008].
For an epidemiologic study, health scientists are interested in information on the probability that a person or population was exposed to a contaminant exceeding a specific concentration level [Suarez-Soto et al., 2008]. For this study, it is the probability that residents of Tarawa Terrace were exposed to drinking water with PCE concentration greater than the 5 ppb MCL. The cumulative probability for the PCE concentration at the WTP exceeding the MCL at a specific time can be found in Figure 5.11. In the figure, the frequency and cumulative probability of PCE MCL arrival at the WTP under Scenario 1 are also compared to a theoretical normal distribution with mean of 86.03 stress periods and standard deviation of 2.74 stress periods. From the figure, it can be concluded that the PCE MCL arrival time distribution for Scenario 1 is very close to a normal distribution.
Another way of finding the probability of exceeding a specific concentration level at a specific time spot is using Figure 5.12. For example, the probability that the PCE concentration at the WTP could exceed the MCL during January 1958 is determined in the following manner:

i. Locate the probabilistic type curve for January 1958 in Figure 5.12;

ii. Locate the 5 ppb MCL on the x-axis;

iii. Follow the vertical line till it intersects with the type curve for January 1958;

iv. Follow the horizontal line till it reaches the y-axis; and

v. Read the probability value on the y-axis.
By using this method, it can be determined that under Scenario 1 the probability for the PCE concentration at the WTP to exceed the 5 ppb MCL during January 1958 is 38.4%, which is same as that can be found in Figure 5.11.

![Figure 5.12. Probability of exceeding concentrations of PCE at the WTP for Scenario 1](image)

5.3.2 MCS Results of Scenario 2

For Scenario 2, 700 realizations were generated for the MCS process, of which 684 simulations were conducted successfully and considered as valid realizations. The relative changes of CV as increasing of the number of realizations are analyzed and plotted in Figure 5.13. As it can be seen from the figure, the MCS converges as the number of realizations is increased to 684, at which point the relative changes of CV
range from -0.288% – 0.393%, and the average of relative changes is decreased to -0.035%.

Figure 5.13. Relative change of CV vs. number of realizations for Scenario 2

Similar to Figure 5.10, analysis of simulation results from the 684 simulations yields the mean and 95% interval of PCE concentration at the WTP as shown in Figure 5.14. Figure 5.14 leads to the following observations:

i. The mean PCE MCL arrival time at the WTP for Scenario 2 is April 1958, which is five months later than the result of the calibrated Camp Lejeune model;
ii. PCE MCL arrival times from 95% of the simulations fall into the range of November 1957 and December 1958, which included the result obtained from the calibrated model (November 1957); and

iii. During January 1985, the PCE concentration at the WTP would vary between 104 – 280 ppb with a probability of 95%. This range includes the calibrated value of 176 ppb and the maximum measured value of 215 ppb, too;

iv. Most part of the PCE concentrations from the calibrated model still lies in the 95% interval, which indicates that the calibrated model is a reasonable representation of the real situation at the site even with the variation of pumping schedules being considered.

Figure 5.14. Statistical results of PCE concentration at the WTP for Scenario 2
Figures 5.15 and 5.16 are similar to Figures 5.11 and 5.12. From these two figures, it can be found that with the variation of pumping schedules being considered, the probability for the PCE concentration at the WTP to exceed the MCL during January 1958 is 11.6%. Another observation one can make from Figure 5.15 is that the PCE MCL arrival times at the WTP for Scenario 2 also closely follow a normal distribution with mean of 87.94 stress periods and standard deviation of 2.78 stress periods.

Figure 5.15. Frequency and cumulative probability of PCE concentration at the WTP exceeding the MCL for Scenario 2
5.3.3. Comparison of MCS Results for Scenario 1 and Scenario 2

According to the discussions of MCS results for Scenario 1 and Scenario 2, the mean values of PCE concentrations at the WTP for both scenarios are quite close to the results obtained from the calibrated Camp Lejeune model, and the PCE MCL arrival times at the WTP for both scenarios closely follow normal distributions. However, further comparisons of the MCS results under two different scenarios reveal that including pumping schedule as an uncertain variable can cause evident changes to the MCS results. Comparison of mean PCE concentrations and PCE MCL arrival times at the WTP for Scenario 1 and Scenario 2 together with the calibrated Camp Lejeune model is shown in Figure 5.17.
The following observations can be made from Figure 5.17:

i. The PCE MCL arrival time under Scenario 2 (April 1958) is five months later than under the calibrated model (November 1957) and two months later than under Scenario 1 (February 1958);

ii. The mean PCE concentration curve for Scenario 2 is not as smooth as those for Scenario 1 and the calibrated model, especially for the time period before 1975. This may be caused by two reasons. One reason is the variations of the historical pumping demands generated for Scenario 2. As can be seen in Figure 5.8, for Scenario 1 and the calibrated model, the total pumping demands for the time period before 1975 were constant. On the contrary, the historical pumping
demands for Scenario 2 are generated by assuming a variation by month. The other reason is the oscillations of the pumping rates in water-supply well TT-26. As one can recall, TT-26 is the most critical well that can cause the change of PCE concentration at the WTP for Camp Lejeune model. The variation of pumping rates in well TT-26 can cause a variation of PCE concentration at the WTP as well. Figure 5.18 demonstrates the comparison of $Q_{TT-26}/Q_{C_{TT-26}}$ values, which are the ratios of pumping rates in well TT-26 to its capacity, for different scenarios. From the figure, it can be seen that for the calibrated model and Scenario 1, the ratios are much more stable, which causes a smoother change of PCE concentrations at the WTP;

iii. The mean PCE concentration curve for Scenario 1 is much closer to that of the calibrated model than for Scenario 2. This is caused by the variations of total pumping demands and pumping rates in well TT-26 under Scenario 2 as well. As one can see in Figure 5.19, the mean values of $Q_{TT-26}/Q_{C_{TT-26}}$ for Scenario 2 remain a constant value of 0.8, while for Scenario 1 the $Q_{TT-26}/Q_{C_{TT-26}}$ values vary through the simulation. Therefore the pumping rates in well TT-26 were higher during some time periods under Scenario 2 than under Scenario 1, while being lower in some other periods. Accordingly, a more significant change of PCE concentrations at the WTP was yielded for Scenario 2. This also explains the reason that the mean PCE MCL arrival time for Scenario 1 is closer to the calibrated model.

The differences discussed above further demonstrate that pumping schedule variation can take significant uncertainties to PCE concentrations and PCE MCL arrival
time at the WTP. Therefore, for the uncertainty analyses conducted for Camp Lejeune model, the analysis results for Scenario 2 are more preferred.

Figure 5.18. Comparison of $Q_{TT-26}/Q_{CT-26}$ for different scenarios
Figure 5.19. Comparison of mean values of $\frac{Q_{TT-26}}{Q_{TT-26}}$ for different scenarios
Figure 5.20. Comparison of probabilities of exceeding concentrations of PCE at the WTP for different scenarios

5.4 Summary

Epidemiologic studies are often retrospective. Due to the limited availability of exposure data, historical reconstructions are used to provide additional exposure information. However, the nature of historical reconstructions determines that there are often uncertainties associated with the constructed input data and thus the results of the simulation models. Therefore, uncertainty analysis is necessary for a reliable and accurate epidemiologic study.

In this chapter, an improved MCS method was applied to evaluate the uncertainties residing in the final results of Camp Lejeune model. In this method, a filtering process is included to ensure the validities of randomly generated realizations.
An embedded statistical module is utilized to improve the computational efficiency of MCS by terminate simulations as soon as the pre-defined stopping criterion is met.

Two improved MCS processes were conducted in this study: Scenario 1 and Scenario 2. The uncertain parameters included in Scenario 1 are: hydraulic conductivities in layers 1, 3, and 5; effective porosity; first order reaction rate; mass loading rate; recharge rate; bulk density; distribution coefficient; and longitudinal dispersivity. To further evaluate the effect of pumping schedule variation on PCE concentrations and PCE MCL arrival times at the WTP, pumping schedule is also included as an uncertain variable for Scenario 2.

According to the analysis results, when pumping schedule variation is not considered, the mean PCE concentrations at the WTP obtained from the MCS study are very close to those obtained from Camp Lejeune model. However, the difference of PCE concentration can be quite significant when pumping schedule variation is taken into consideration.

The uncertainty analyses results for the two scenarios also conclude that:

i. The PCE concentrations obtained from the calibrated Camp Lejeune model are reasonable;

ii. The most probable time for the PCE concentration at Tarawa Terrace WTP to exceed MCL is end of year 1957 and beginning of year 1958; and

iii. Pumping schedule variation can cause significant change of PCE concentrations and PCE MCL arrival time at Tarawa Terrace WTP.
CHAPTER 6

EVALUATION OF CONTAMINANT ARRIVAL TIMES UNDER MULTI-PARAMETER UNCERTAINTIES

6.1 Introduction

Studies described in Chapters 4 and 5 demonstrate that uncertainties associated with the input data of groundwater flow and contaminant fate-and-transport models can take significant uncertainties to the simulation results such as contaminant concentration and arrival time, which in turn can seriously impact the reliability of the related epidemiologic studies. PSOpS developed in Chapter 4 can efficiently quantify the uncertainties associated with the arrival time caused by pumping schedule variations. It works by optimizing pumping schedule and using it as input in a contaminant transport simulation model to obtain extreme contaminant arrival times (i.e., earliest and latest arrival times).

A reliable epidemiologic study sometimes may require the evaluation of extreme contaminant arrival times at an exposure point under multi-parameter uncertainties in addition to pumping schedule variations. A possible solution to this problem is applying PSOpS to a set of equally probable realizations generated according to probabilistic distributions of the uncertain parameters. The extreme contaminant arrival times under multi-parameter uncertainties can then be obtained by comparing the resulting extreme arrival times for each individual realization. In this manner, the problem is turned into a stochastic optimization problem.
Stochastic optimization under uncertainties has become a very important research area in recent years. In comparison with a deterministic optimization, a stochastic optimization considers some or all of the system input parameters as stochastic or uncertain variables [Bakr et al., 2003]. The statistical method is a major approach for the solution of stochastic optimization problems. It generates a set of equally probable realizations according to the probabilistic distribution of uncertain parameters using statistical techniques to represent the effect of uncertainties. Its basic idea is that the more realizations a solution complies with, the more robust the outcome will be. This approach has been widely applied to groundwater quality management problems with uncertainties [Aly and Peralta, 1999; Bau and Mayer, 2006; Chan, 1994; Hilton and Culver, 2005; Mantoglou and Kourakos, 2007; Mylopoulos et al., 1999; Smalley et al., 2000; Wagner and Gorelick, 1989; Wagner et al., 1992].

Usually, the reliability of the stochastic optimization results improves as the number of realizations used in the optimization process increases due to better representation of parameter uncertainties with increased number of realizations. However, this reliability improvement is associated with significant increase in computational cost, especially for field-scale problems. The previous studies on the subject have shown that although each realization is equally probable during a stochastic optimization, the effects they have on the final optimization results can be quite different – only a few realizations are really critical to the final results, which are thereby called “critical realizations” [Mantoglou and Kourakos, 2007; Ranjithan et al., 1993]. Apparently, the application of only a few critical realizations in the optimization process
instead of the whole set of realizations can dramatically improve the computational efficiency while maintaining a desired reliability level.

In Ranjithan et al. [1993], the critical realizations were used to improve the computational efficiency for optimal remediation design where uncertainty associated with the hydraulic conductivity parameter was considered. The level of criticalness of each realization, which was determined by the spatial distribution and the degree of variation of the hydraulic conductivity values, was identified using the pattern classification capability of neural networks. While the authors have demonstrated the reliability and efficiency of the optimal remediation design using critical realizations, this work only considered the uncertainty associated with the hydraulic conductivities. The pattern classification technique restricts the application of this method to problems with uncertain parameters showing no clear patterns, such as pumping schedule, or problems with multiple uncertain parameters. Furthermore, training of neural networks may be quite computationally intensive, and may potentially lower the efficiency of this method.

In the optimal pump-and-treat system design methodology developed by Mantoglou and Kourakos [2007], the objective function values of the realizations under various remediation policies were evaluated and ranked. The critical realizations were then selected based on their ranks. Application of this method to an example problem shows that a few critical realizations could retain a comparable reliability level in optimal remediation design while reducing the computational demand significantly. However, the authors also considered the hydraulic conductivity to be the only uncertain variable.

In this chapter, a quantitative procedure named Pareto Dominance based Critical Realization Identification (PDCRI) was developed to screen out critical realizations under
multi-parameter uncertainties by using Pareto dominance analysis, so that evaluation of extreme contaminant arrival times can be accomplished in an efficient manner – by applying PSOpS to the few critical realizations in stead of a large number of equally likely realizations can significantly reduce the computational demand while maintaining a similar level of reliability. The effectiveness and reliability of PDCRI was first illustrated by a hypothetical example. PDCRI and PSOpS were then applied together to evaluate the extreme contaminant arrival times under multi-parameter uncertainties for Camp Lejeune model.

### 6.2 Methodology of PDCRI

The Pareto Dominance based Critical Realization Identification (PDCRI) is a procedure that uses Pareto dominance analysis to identify critical realizations for stochastic optimization problems with single or multiple parameter uncertainties. Prior to description of the detailed procure, a few terms used in PDCRI are explained as they are defined in this study.

**Realization:** A realization is a set of uncertain parameters that are generated for one contaminant transport simulation. Realizations are usually generated from the probabilistic model of uncertain parameters using statistical techniques.

**Critical realization:** Critical realizations are realizations that can yield the extreme contaminant arrival times with high reliabilities.

**Scenario:** A scenario is usually a set of decision variables of the related optimization problem. For this study, a scenario stands for a pumping schedule.

**Objective:** Objective is the system response to a realization and a scenario. The objective in this study is the contaminant concentration at the exposure point.
**Reliability:** The reliability of a realization is defined as the probability that the extreme arrival time derived from the realization is the closest overall extreme arrival time considering parameter uncertainties.

**Pareto dominance:** The Pareto dominance is one of the key notions in multi-objective optimization problems [Voorneveld, 2003]. Considering two real $n$-dimensional vectors \( \{x\} \) and \( \{y\} \), if all the coordinates of vector \( \{x\} \) are equal or better than the coordinates of vector \( \{y\} \), with at least one coordinate being strictly better, then vector \( \{x\} \) is said to Pareto dominate vector \( \{y\} \), and vector \( \{y\} \) is dominated by vector \( \{x\} \) [Voorneveld, 2003]. Figure 6.1 illustrates the Pareto dominance in a two-objective optimization problem, where \( x_1 \) and \( x_3 \) dominate \( x_2 \), or say \( x_2 \) is dominated by \( x_1 \) and \( x_3 \), but \( x_1 \) and \( x_3 \) are not dominated by each other. In a PDCRI application, the criticalness of a realization is evaluated by Pareto dominance analysis.

![Figure 6.1. Illustration of Pareto dominance](image-url)
The working procedure of PSOpS is illustrated in Figure 6.2. In the first step, a large set of equally probable realizations are generated based on the given probability distributions of uncertain parameters. Several pumping schedules (i.e., scenarios) are also randomly generated according to pumping capacities of the candidate wells. The objective value with regard to each realization under each scenario is then evaluated by using groundwater flow and contaminant transport simulation models. Assuming that \( n \) realizations and \( m \) scenarios are generated during a PDCRI application, a total number of \( mn \) groundwater flow and contaminant transport simulations will be conducted. By using objective values obtained from the simulations, an objective vector will be formed for each realization, which consists of \( m \) objective values.

![Figure 6.2. Flowchart of PDCRI](image)

After the \( n \) objective vectors are obtained, a Pareto dominance analysis is conducted on these objective vectors to determine the number of times that each objective vector dominates and is dominated with respect to other objective vectors. According to the Pareto dominance analysis results, a quantitative index identified as Criticalness Index (CI) can be calculated to indicate the criticalness of a realization. CI is defined by the following equation:

\[
CI_i = \frac{J_i}{n-1} + \frac{n-1 - J_i - K_i}{(n-1)(n-J_i)},
\]

(6.1)
where CI$_i$ is the CI value for realization $i$; $n$ is the total number of realizations used in PDCRI; $J_i$ is the number of times the objective vector of realization $i$ dominates others; and $K_i$ is the number of times that the objective function vector of realization $i$ is dominated. By this definition, the values of CI vary between 0 and 1. A realization with CI = 1 is the most critical one, and a realization with CI = 0 is the least critical one.

In Equation (6.1), the term $J_i/(n-1)$ makes up the major part of a CI value. It indicates that for the $n$ realizations used in a PDCRI application, the more times the objective vector of a realization dominates, the closer the CI value is to 1, and the more critical the realization is. The basic idea is that, if a realization has more chances to yield higher contaminant concentrations under multiple pumping schedules, the distribution of hydrogeologic parameters used in this realization can facilitate faster movement of contaminant, that is, the hydrogeologic parameter realization has a better chance to yield the earliest contaminant arrival time under the optimal pumping schedule. Similarly, it is very likely that the latest arrival time can be obtained from a realization that always yields lower contaminant concentrations under various pumping scenarios.

The term $(n-1-J_i-K_i)/[(n-1)(n-J_i)]$ in Equation (6.1) is used to compare the criticalness of realizations with same $J_i$ values. In such a case, a higher CI value will be obtained for the realization with less number of times being dominated by others, implying that it is more critical. It must be point out that according to Equation (6.1), a realization whose objective vector dominating $J_i$ times is never able to obtain a CI value greater than $(J_i+1)/(n-1)$ no matter how many times its objective vector is dominated, indicating that the number of times that an objective vector dominates is the major factor in CI value calculation. As an example, given a case with 100 realizations, if the
objective vector of a realization dominates 75 times and is dominated 10 times, the CI value of this realization is

$$CI = \frac{75}{100-1} + \frac{100 - 1 - 75 - 10}{(100 - 1)(100 - 75)} = 0.763.$$  \hspace{1cm} (6.2)

After the CI value for each realization is obtained, the critical realizations can be picked up for the optimization process according to CI values and reliability requirement of the related stochastic optimization problem. As can be seen in later discussions, the reliability of a realization is very close to its CI value if the CI value is close 1. In other words, if the optimization result for a stochastic optimization problem is obtained by using a critical realization with \( CI = \alpha \), then the probability for the result to be the “true” optimal is very close to \( \alpha \). Therefore, if a stochastic optimization problem desires optimal solution with a possibility of at least \( \alpha \), realizations with CI values of \( \alpha \) or higher should be chosen as critical realizations.

### 6.3 Verification of PDCRI

To demonstrate the effectiveness and reliability of PDCRI, a hypothetical application with uncertain hydraulic conductivities was created. As shown in Figure 6.3, the unconfined aquifer is bounded by no-flow boundaries to its North and South. The east and west boundaries are constant head boundaries with heads of 36 feet and 40 feet, respectively. The dimensions of the site are 2,700 feet \( \times \) 2,000 feet \( \times \) 50 feet, which is simulated using 270 columns, 200 rows, and 1 layer in MODFLOW and MT3DMS. Each cell has the same size of 10 feet \( \times \) 10 feet \( \times \) 50 feet. For the groundwater flow and contaminant transport simulations, each month is simulated as one stress period. Starting from time zero, contaminant is released to the aquifer from node (100, 70) at a constant
rate of 100 g/day. As indicated in Figure 6.3, the contaminant is then collected by the candidate wells with a pumping capacity of 3,000 ft$^3$/day in each well at a total water supply of 7,000 ft$^3$/day. The goal of the example problem is to evaluate the earliest contaminant maximum contaminant level (MCL, 20 ppb for the example contaminant) arrival time in the discharged water based on hydraulic conductivity uncertainties. The various hydraulic conductivity distributions were generated using FIELDGEN [Doherty, 2007]. One example realization of the hydraulic conductivity distributions is shown in Figure 6.3. Other properties of the site and the contaminant used in this example are given in Table 6.1.

Figure 6.3. The candidate well locations, contaminant source, hydraulic conductivity and initial head distributions for the example problem (hydraulic conductivity unit: ft/day, head unit: ft)
Table 6.1. Values of parameters used in the example problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquifer thickness</td>
<td>50 ft</td>
</tr>
<tr>
<td>Aquifer specific yield</td>
<td>0.05</td>
</tr>
<tr>
<td>Effective porosity</td>
<td>0.2</td>
</tr>
<tr>
<td>Longitudinal dispersivity</td>
<td>25 ft</td>
</tr>
<tr>
<td>Horizontal transverse dispersivity</td>
<td>2.5 ft</td>
</tr>
<tr>
<td>Vertical transverse dispersivity</td>
<td>0.25 ft</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>$8.5 \times 10^{-4}$ ft$^2$/day</td>
</tr>
<tr>
<td>Soil bulk density</td>
<td>$7.7112 \times 10^4$ g/ft$^3$</td>
</tr>
<tr>
<td>Distribution coefficient</td>
<td>$5.0 \times 10^{-6}$ ft$^3$/g</td>
</tr>
<tr>
<td>Contaminant first order reaction rate</td>
<td>$5.0 \times 10^{-4}$ 1/day</td>
</tr>
</tbody>
</table>

For an accurate evaluation of the reliability of stochastic optimization using critical realizations, the probability distribution of the earliest MCL arrival times under hydraulic conductivity uncertainties were pre-obtained using MCS. During the MCS, the earliest MCL arrival times for 1,100 realizations were calculated by using PSOpS. As indicated in Figure 6.4, the cumulative probability distribution for the earliest contaminant MCL arrival times is very close to that of a theoretical normal distribution with mean of 8.505 stress periods and standard deviation of 0.277 stress periods, which is therefore taken as the “true” distribution of the earliest MCL arrival times.

To study the reliability improvement of critical realizations with regard to the number of realizations and number of scenarios used in PDCRI, another 1,000 realizations were generated for the example problem. For each realization, the contaminant concentrations in the discharge at the end of stress period 5 under 10 different pumping schedules were evaluated and then used for CI calculations as discussed below.
6.3.1 Improvement of Reliability vs. Number of Realizations

In our study, the CI values under 10 scenarios were calculated for various numbers of realizations ($N_T$) as indicated in Table 6.2 to examine the reliability of the critical realizations with regard to the total number of realizations used in PDCRI. The obtained CI value and reliability of each realization are plotted in Figure 6.5 for cases with 10, 100, and 1,000 realizations, respectively. For the example problem, the reliability of each realization is calculated by using the cumulative probability of the earliest arrival time under the “true” distribution to subtract 1. It can be seen from Figure 6.5 that as the CI value of a realization approaches 1, the reliability of the realization is...
quite close to its CI value. The higher is the CI value of a realization, the higher is the probability that the realization can yield the earliest MCL arrival time, which demonstrates the effectiveness of criticalness indication using CI.

Table 6.2. Reliabilities of critical realizations with CI values greater than 0.90 and 0.95 for the example problem

<table>
<thead>
<tr>
<th>N_T</th>
<th>N_CI90</th>
<th>N_P90</th>
<th>N_P90/ N_CI90 (%)</th>
<th>N_CI95</th>
<th>N_P95</th>
<th>N_P95/ N_CI95 (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1</td>
<td>1</td>
<td>100</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>1</td>
<td>50</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>50</td>
<td>2</td>
<td>2</td>
<td>100</td>
<td>2</td>
<td>1</td>
<td>50</td>
</tr>
<tr>
<td>100</td>
<td>3</td>
<td>3</td>
<td>100</td>
<td>1</td>
<td>1</td>
<td>100</td>
</tr>
<tr>
<td>200</td>
<td>5</td>
<td>5</td>
<td>100</td>
<td>3</td>
<td>3</td>
<td>100</td>
</tr>
<tr>
<td>300</td>
<td>8</td>
<td>8</td>
<td>100</td>
<td>4</td>
<td>4</td>
<td>100</td>
</tr>
<tr>
<td>400</td>
<td>13</td>
<td>12</td>
<td>92</td>
<td>7</td>
<td>7</td>
<td>100</td>
</tr>
<tr>
<td>500</td>
<td>18</td>
<td>17</td>
<td>94</td>
<td>8</td>
<td>8</td>
<td>100</td>
</tr>
<tr>
<td>600</td>
<td>20</td>
<td>19</td>
<td>95</td>
<td>9</td>
<td>9</td>
<td>100</td>
</tr>
<tr>
<td>700</td>
<td>23</td>
<td>22</td>
<td>96</td>
<td>12</td>
<td>12</td>
<td>100</td>
</tr>
<tr>
<td>800</td>
<td>28</td>
<td>27</td>
<td>96</td>
<td>14</td>
<td>13</td>
<td>93</td>
</tr>
<tr>
<td>900</td>
<td>30</td>
<td>29</td>
<td>97</td>
<td>15</td>
<td>13</td>
<td>87</td>
</tr>
<tr>
<td>1000</td>
<td>35</td>
<td>34</td>
<td>97</td>
<td>18</td>
<td>16</td>
<td>89</td>
</tr>
</tbody>
</table>

Data listed in Table 6.2 provide information for further investigation of the relationship between the CI values and the reliabilities of critical realizations obtained by PDCRI using various numbers of realizations. In the table, N_CIlm indicates the number of critical realizations with CI values greater than m%, while N_Pm indicates the number of critical realizations among the N_CIlm ones that can yield earliest MCL arrival times with reliabilities higher than m%. It can be seen from Table 6.2 that a PDCRI application using a small number of realizations is not able to provide critical realizations with high reliabilities. For example, at least 50 realizations are required to find realizations with reliabilities higher than 95%. As the number of realizations used in PDCRI increases,
more critical realizations with high reliabilities can be screened out. It is because that, with more realizations used in PDCRI, the effect of parameter uncertainties can be expressed more thoroughly, thus realizations can be found to represent more critical situations. In other words, the reliabilities of critical realizations can be improved by increasing the number of realizations used in PDCRI.

The \( N_{pm} \) to \( N_{Clm} \) ratios given in Table 6.2 demonstrate that most critical realizations with high CI values have reliabilities no less than the CI values. In other words, for the example problem, one can usually expect an earliest MCL arrival time with a reliability of at least \( \alpha \) by using critical realizations with CI values larger than \( \alpha \).

Figure 6.5. Criticalness Indexes vs. reliabilities of realizations used in PDCRI

![Figure 6.5. Criticalness Indexes vs. reliabilities of realizations used in PDCRI](image)
Regressions of data listed in Table 6.2 are illustrated in Figure 6.6. The figure tells that, for the example problem, the number of realizations with CI values higher than a specific value increases linearly as the number of realizations used in PDCRI. Interestingly, only about 3.4% of all realizations have CI values higher than 0.90, but half of these realizations have CI values higher than 0.95. Therefore, if one wants to find \( n \) critical realizations that can provide stochastic optimization results with reliabilities higher than 0.95, a minimum number of \( n/0.017 \) realizations should be generated for the PDCRI. This number may vary for different problems. Nevertheless, as a general rule, the more critical realizations and higher reliabilities are pursued, the larger number of realizations should be used in PDCRI.

![Figure 6.6. Number of realizations with CI values greater than 0.90 and 0.95 for PDCRI applications with various numbers of realizations](image-url)
6.3.2 Improvement of Reliability vs. Number of Scenarios

Pareto dominance analysis is used to compare multi-objective vectors. Therefore, at least two different scenarios are required in PDCRI. To analyze the reliability improvement caused by increasing the number of scenarios used in PDCRI, PDCRI was conducted with various number of realizations as listed in Table 6.3 under 2 – 10 different pumping schedules to identify critical realizations for the example problem. To quantify the improvement of reliability, a term named refreshment rate, RR_{m,n}, is defined as the percentage of realizations refreshed among the first n% most critical realizations when the number of scenarios used in PDCRI is increased from (m-1) to m. For instance, if a total of 500 realizations are used in PDCRI, when the number of scenarios is increased from 2 to 3, there are 1 realization changed in the top 3% most critical realizations, the RR_{3,3} is then calculated as \(\frac{1}{(500 \times 3\%) \times 100\%} = 6.67\%\).

<table>
<thead>
<tr>
<th>Number of Realizations</th>
<th>RR_{2,3}</th>
<th>RR_{3,3}</th>
<th>RR_{4,3}</th>
<th>RR_{5,3}</th>
<th>RR_{6,3}</th>
<th>RR_{7,3}</th>
<th>RR_{8,3}</th>
<th>RR_{9,3}</th>
<th>RR_{10,3}</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>26.67</td>
<td>6.67</td>
<td>6.67</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>600</td>
<td>22.22</td>
<td>0</td>
<td>0</td>
<td>5.56</td>
<td>5.56</td>
<td>0</td>
<td>5.56</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>700</td>
<td>23.81</td>
<td>4.76</td>
<td>0</td>
<td>4.76</td>
<td>4.76</td>
<td>4.76</td>
<td>9.52</td>
<td>4.76</td>
<td>0</td>
</tr>
<tr>
<td>800</td>
<td>20.83</td>
<td>0</td>
<td>0</td>
<td>8.33</td>
<td>8.33</td>
<td>0</td>
<td>8.33</td>
<td>4.17</td>
<td>0</td>
</tr>
<tr>
<td>900</td>
<td>29.63</td>
<td>3.70</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.70</td>
<td>7.41</td>
<td>0</td>
</tr>
<tr>
<td>1,000</td>
<td>26.67</td>
<td>3.33</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6.67</td>
<td>6.67</td>
<td>0</td>
</tr>
</tbody>
</table>

The refreshment rates for the example problem with various numbers of realizations and scenarios are calculated and given in Table 6.3. As it is discussed before, a PDCRI application requires at least two scenarios. Therefore, the RR_{2,3} values in the table are solely for comparison purposes, and the top 3% critical realizations under one
scenario are obtained by finding realizations with the first 3% highest contaminant concentrations under a single pumping schedule in stead of using PDCRI. It can be observed from the table that when the number of scenarios is changed from 1 to 2, the refreshment rates are always higher than 20%, which means that more than 20% of the top 3% critical realizations are changed. This validates the usage of multi-objective Pareto dominance analysis for critical realization identification in PDCRI. However, it can also be seen from Table 6.3 that, when the number of scenarios increases from 2, the refreshment rates are relatively small. In other words, the top 3% critical realization lists are quite stable. Comparing to the discussion in the previous section, this observation indicates that the number of realizations is more important than the number of scenarios for a PDCRI procedure. To obtain more reliable critical realizations, the number of realizations should be increased in stead of the number of scenarios.

### 6.4 Application of PDCRI to Camp Lejeune Model

To evaluate the extreme PCE MCL arrival times at Tarawa Terrace WTP under multi-parameter uncertainties, PDCRI was first applied to screen out the few critical realizations for extreme arrival times. Application of PSOpS to these critical realizations then yielded extreme arrival times with high reliabilities while maintaining relatively low computational cost.

The resulting extreme PCE MCL arrival times consider the effects of all the critical uncertain variables as identified in Chapter 3, which include hydraulic conductivities in aquifer layers 1, 3, and 5; bulk densities and effective porosities of the porous media; the first order reaction rate, mass loading rate, distribution coefficient, and longitudinal dispersivity of PCE; the recharge rate; and the pumping schedule at the
Camp Lejeune site. During the PDCRI application, realizations were generated according to the probabilistic distributions of all uncertain factors mentioned above but pumping schedules because the uncertainties caused by pumping schedule would be reflected during PSOpS optimizations.

During the PDCRI application, it was constantly observed that the top 1.5% critical realizations had CI values greater than 0.985. It was also observed that increasing the number of scenarios, again, led to very low refreshment rates. Therefore, a total number of 700 realizations and 2 scenarios were employed in this study to provide 10 critical realizations with CI values higher than 0.985. The resulting concentration vectors were evaluated twice by using Pareto dominance analysis – one for earliest MCL arrival times (high concentration) and the other for latest ones (low concentration), based on which the CI values with regard to these two objectives were calculated.

According to the CI values, 10 critical realizations were identified for earliest and latest PCE MCL arrival times, respectively. Application of PSOpS to these critical realizations yielded the earliest arrival time of July 1956, and the latest arrival time of July 1961. Compared to the extreme arrival times under pumping schedule uncertainties only (December 1956 and June 1960), the extreme arrival time interval is expanded by another 18 months. Considering that the CI values of the critical realizations are higher than 0.985, reliabilities of the results of both sides are about 98.5%, too. And it can be concluded that, under multiple parameter uncertainties, the PCE MCL arrival time at the Tarawa Terrace WTP varies between July 1956 and July 1961 with a reliability of no less than 97%.
According to the discussion in Chapter 4, as the major contributor of PCE to the Tarawa Terrace WTP, well TT-26 pumped at its capacities under the Maximum Schedule, and pumped at its lowest possible rates most of the time under the Minimum Schedule I. Therefore, the Maximum Schedule and the Minimum Schedule I are also very possible the optimal schedules for the other realizations that can yield the earliest and latest PCE MCL arrival times at the WTP. In other words, the probability distributions of PCE MCL arrival times obtained under the Maximum Schedule and the Minimum Schedule I are quite close to the probability distributions of the earliest and latest PCE MCL arrival times under uncertainties. The two cumulative probability distributions and their corresponding theoretical distributions are illustrated in Figures 6.7 and 6.8, together with the earliest and latest arrival times obtained by using the critical realizations. From the figures, one can tell that the reliabilities of the results discussed above are actually higher than expected, which proves the validity of critical realizations identified by PDCRI.
Figure 6.7. Cumulative probabilities of MCL arrival for critical realizations under the Maximum Schedule
Figure 6.8. Cumulative probabilities of MCL arrival for critical realizations under Minimum Schedule I

6.5 Summary

Uncertainties associated with the input data of groundwater flow and contaminant fate-and-transport models can take significant uncertainties to the simulation results such as contaminant concentration and arrival time, which in turn can seriously impact the reliability of the related epidemiologic studies. Therefore, a reliable epidemiologic study sometimes requires the evaluation of extreme contaminant arrival times under multi-parameter uncertainties in addition to pumping schedule variations.

The model complexity and huge computational demand associated with field-scale problems such as Camp Lejeune model prohibit the application of traditional
uncertainty analysis and optimization methods on such evaluations. Therefore, in this chapter, a procedure named Pareto Dominance based Critical Realization Identification (PDCRI) was developed to cope with PSOpS, so that evaluation of extreme contaminant arrival times under multi-parameter uncertainties can be accomplished in a timely manner.

The effectiveness and reliabilities of the critical realizations obtained by using PDCRI were tested using a hypothetical example. Optimization results indicate that application of critical realizations in stochastic optimization problems can significantly improve the computational efficiency while maintaining a similar reliability. An optimization problem using critical realizations can yield results with reliabilities close to their CI values.

It is also demonstrated that the reliabilities of critical realizations will improve as the number of realizations used in PDCRI increases. Two different scenarios are necessary for PDCRI as the reliabilities of the critical realizations can be improved obviously. However, use of more than two scenarios in PDCRI will not improve the reliabilities of the critical realizations quite much. As a general rule, more realizations in stead of scenarios should be generated for PDCRI if highly reliable critical realizations are pursued.

Combinational application of PDCRI and PSOpS on Camp Lejeune model successfully provided a PCE MCL arrival time interval with 97% reliability by using only 20 critical realizations. It shows that the PDCRI procedure is reliable and suitable for field-scale problems with multi-parameter uncertainties and may be applied to other
groundwater quality management problems with multiple parameter uncertainties to improve computational efficiency.
CHAPTER 7

CONCLUSIONS

Exposures of human beings to environmental contaminants might cause serious health effects. An epidemiologic study is a method used by health scientists to reveal these relationships. In retrospective epidemiologic studies, quantitative historical information is often too limited for exposure assessment. One way to fill the data gap is historical reconstruction and simulation analyses [Maslia et al., 2003; Nieuwenhuijsen et al., 2006]. Due to the nature of the historical reconstruction process, there are inevitably uncertainties associated with the input data and, therefore, with the final results of the simulation models, potentially adversely impacting related epidemiologic investigations.

Evaluation of uncertainties residing in the final results can provide invaluable supportive information for the related health study. Owing to the fact that historically reconstructed simulation models for epidemiologic studies are often field-scale complex models, uncertainty analysis regarding such simulations models can be computationally intensive.

In this study, several procedures were developed to improve computational efficiency for uncertainty analysis of contaminant fate and transport in a field-scale subsurface system. These procedures were then used in a site specific application conducted at U.S. Marine Corps Base Camp Lejeune, North Carolina.

U.S. Marine Corps Base Camp Lejeune is located near Jacksonville, Onslow County, North Carolina. The Agency for Toxic Substances and Disease Registry (ATSDR), U. S. Department of Health and Human Services, is conducting an
epidemiologic study at this site to determine if exposure to contaminated drinking water is related to birth defects and childhood cancer in children born to women who lived on base during the period 1968-1985 [Maslia et al., 2007a].

Due to the limited exposure data available for the epidemiologic study, a large-size simulation model (i.e., Camp Lejeune model) was constructed using MODFLOW and MT3DMS to simulate PCE concentrations at the Tarawa Terrace water treatment plant (WTP) on the base. Because the simulation models were constructed based on very limited information, uncertainty analysis of PCE concentrations and PCE MCL arrival times at Tarawa Terrace WTP are conducted to improve reliability of the epidemiologic study.

Prior to the uncertainty analysis, sensitivity analyses regarding uncertain input parameters were performed to screen out variables that took the most uncertainties into the final simulation results. During the sensitivity analyses, several values for each uncertain parameter were selected within its nominal range for contaminant transport simulations, and the resulting changes of PCE concentrations and PCE MCL arrival times at the WTP were evaluated. The critical uncertain variables that caused the most changes include: hydraulic conductivities in layers 1, 3, and 5; effective porosity; first order reaction rate; mass loading rate; recharge rate; bulk density; distribution coefficient; and longitudinal dispersivity.

The effects of pumping schedule variation on PCE concentrations and PCE MCL arrival times at the WTP were not evaluated during the sensitivity analysis because of the fact that, manipulation of the pumping schedule even without the change of total pumping demand can still cause significant change in groundwater flow and contaminant
fate-and-transport. In this study, to efficiently quantify the uncertainty effect of pumping schedule variation, a procedure identified as Pumping Schedule Optimization System (PSOpS) was developed to evaluate the extreme changes of PCE MCL arrival time at the WTP by employing a simulation/optimization (S/O) approach. Two improved nonlinear programming methods – Rank-and-Assign (RAA) and Improved Gradient (IG) – are used in PSOpS to provide computational efficiency. The improvement of the computational efficiency is achieved by following means:

**The reduction of the dimension of the optimization problem:** By reformulating the optimization problem, the pumping schedule of only the current stress period instead of the current and all previous stress periods needs to be optimized for the optimum contaminant concentration, which makes the dimension of the problem to a computationally manageable magnitude. Utilization of IG optimization method can reduce the dimension of the problem as well by eliminating pumping wells with equal ranks;

**The reduction of the number of iterations:** As the major optimizer of PSOpS, the RAA method usually converges within two iterations, which means less objective function evaluation and much less computational demand; and,

**Elimination of repeated simulations:** Using the piezometric head and concentration distributions under the optimum pumping schedule of the previous stress period as the initial condition eliminates the need of repeated computationally-expensive groundwater flow and contaminant transport simulations.

Application of PSOpS toward Camp Lejeune model demonstrates that pumping schedule variation can cause significant changes in PCE concentrations and PCE MCL
arrival times at the WTP – a close look at the simulation results reveals that the PCE MCL arrival time at the WTP could vary from December 1956 to June 1960.

Various uncertainty analysis methods exist in literature, such as analytical uncertainty analysis methods and Taylor series expansion method. However, application of these methods toward Camp Lejeune model is prohibitive due to the large size and complexity of the model. Therefore, an improved Monte Carlo simulation (MCS) method was applied for uncertainty evaluations. The MCS method applied in this study are majorly improved by two means: (i) a filtering process is adopted to ensure the reliability of realizations and, thus, the final results; and (ii) a statistical module is utilized to terminate the MCS as soon as the stopping criterion is met, so that computational efficiency can be improved.

To further demonstrate the effect of pumping schedule variation on PCE concentrations and MCL arrival times at the WTP, MCS processes were conducted twice in this study under two different scenarios: Scenario 1 and Scenario 2, in which pumping schedule was excluded and included as uncertain variable, respectively.

According to the uncertainty analysis results, when effect of pumping schedule variation is not considered, the mean PCE concentrations at the WTP obtained by MCS are very close to those obtained from the original model. However, evident difference in PCE concentration can be observed when pumping schedule variation is taken into consideration.

Epidemiologic study sometimes requires the evaluation of extreme contaminant arrival times at an exposure point under multi-parameter uncertainties. The model complexity and huge computational demand associated with field-scale problems such as
Camp Lejeune model prohibit the application of traditional uncertainty analysis and optimization methods on such evaluations. In this study, a procedure named Pareto Dominance based Critical Realization Identification (PDCRI) was developed to cope with PSOpS, so that evaluation of extreme contaminant arrival times under multi-parameter uncertainties can be accomplished in a timely manner – by applying PSOpS to the few critical realizations (i.e., realizations that are critical to final numerical results) in stead of a large number of equally likely realizations can significantly reduce the computational demand while maintaining a similar level of reliability. Application of PDCRI to an example problem indicates that critical realizations can provide reliable estimates of extreme contaminant arrival times. Reliability of the critical realizations can be improved by including more realizations in the PDCRI application. Combinational application of PDCRI and PSOpS on Camp Lejeune model reveals that, considering the effect of multi-parameter uncertainties, at least 97% of the extreme PCE MCL arrival times fall into the range of July 1956 to July 1961.
APPENDIX A

PROOF OF RAA METHOD RESULTS SATISFYING KUHN-TUCKER CONDITIONS

Kuhn-Tucker Conditions

The Kuhn-Tucker conditions [Kuhn and Tucker, 1951] are described as follows.

Consider the problem:

\[
\begin{align*}
\text{Min} & \quad f(x) \\
\text{s.t.} & \quad g_i(x) \leq 0 \quad i = 1, \ldots, m \\
& \quad h_j(x) = 0 \quad j = 1, \ldots, l
\end{align*}
\]

(A.1)

where \( g_i(x) \) \((i = 1, \ldots, m)\) is the non-equality constraints; \( h_j(x) \) \((j = 1, \ldots, l)\) is the equality constraints; \( m \) is the number of non-equality constraints; and, \( l \) is the number of equality constraints.

Suppose that the objective function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) and the constraint functions \( g_i : \mathbb{R}^n \rightarrow \mathbb{R} \) and \( h_j : \mathbb{R}^n \rightarrow \mathbb{R} \) are continuously differentiable at a point \( x^* \in S \). If \( x^* \) is a local minimum, then constants \( \lambda_i \geq 0 \) \((i = 1, \ldots, m)\) and \( \mu_j \) \((j = 1, \ldots, l)\) exist such that

\[
\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x^*) + \sum_{j=1}^{l} \mu_j \nabla h_j(x^*) = 0
\]

(A.2)

\[
\lambda_i g_i(x^*) = 0 \text{ for all } i = 1, \ldots, m
\]

Proof of RAA Method Results Satisfying Kuhn-Tucker Conditions

To prove that a solution from the RAA method satisfies the Kuhn-Tucker conditions, the optimization formulation for maximum contaminant concentration at any stress period can be reformulated as:

219
\[
\begin{align*}
\text{Min } & -C = -f(q) \\
\text{s.t.} & \\
-q_i & \leq 0 \ (i = 1, \ldots, n), \\
q_i - w_i & \leq 0 \ (i = 1, \ldots, n) \\
\sum_{i=1}^{n} q_i - Q_T & = 0
\end{align*}
\]  
(A.3)

where \( C \) is the contaminant concentration, which is a function of \( q \); \( n \) is the number of active water-supply wells; \( q \) is an \( n \)-dimensional vector of pumping rates; \( q_i \) is the pumping rate of well \( i \); \( w_i \) is the pumping capacity for well \( i \); and, \( Q_T \) is the total water demand.

The Kuhn-Tucker conditions for the problem given in Equation (A.3) are

\[
\begin{align*}
-\frac{\partial f}{\partial q_i} - \lambda_i + \omega_i + \mu &= 0 \ (i = 1, \ldots, n) \\
\lambda_i q_i &= 0 \ (i = 1, \ldots, n) \\
\omega_i (q_i - w_i) &= 0 \ (i = 1, \ldots, n) \\
\lambda_i &\geq 0 \ (i = 1, \ldots, n) \\
\omega_i &\geq 0 \ (i = 1, \ldots, n)
\end{align*}
\]  
(A.4)

Suppose the optimal solution from the RAA method is

\[
q_i \begin{cases} 
= w_i & (i = 1, \ldots, k - 1) \\
\leq w_i & (i = k) \\
= 0 & (i = k + 1, \ldots, n)
\end{cases}
\]  
(A.5)

while the following condition is satisfied,

\[
\frac{\partial f}{\partial q_1} \geq \ldots \geq \frac{\partial f}{\partial q_k} \geq \ldots \geq \frac{\partial f}{\partial q_n}.
\]  
(A.6)

For \( i \leq k \), since \( q_i > 0 \), to satisfy \( \lambda_i q_i = 0 \), there is:

\[
\lambda_i = 0 \ (i = 1, \ldots, k).
\]  
(A.7)

According to equation: \(-\frac{\partial f}{\partial q_i} - \lambda_i + \omega_i + \mu = 0\), there is:
\[ \omega_i = \frac{\partial f}{\partial q_i} - \mu \ (i = 1, \ldots, k) . \] (A.8)

Let \( \mu = \frac{\partial f}{\partial q_k} \), there is:

\[ \omega_k = 0 . \] (A.9)

Since \( \frac{\partial f}{\partial q_i} \geq \frac{\partial f}{\partial q_k} \) for \( i < k \), there is:

\[ \omega_i = \frac{\partial f}{\partial q_i} - \frac{\partial f}{\partial q_k} \geq 0 \ (i = 1, \ldots, k - 1) . \] (A.10)

For \( i > k \), since \( q_i = 0 \), to satisfy \( \omega_i (q_i - w_i) = 0 \), there must be:

\[ \omega_i = 0 \ (i = k + 1, \ldots, n) . \] (A.11)

According to equation \(-\frac{\partial f}{\partial q_i} - \lambda_i = \omega_i + \mu = 0 \) there is:

\[ \lambda_i = \mu - \frac{\partial f}{\partial q_i} = \frac{\partial f}{\partial q_k} - \frac{\partial f}{\partial q_i} \ (i = k + 1, \ldots, n) . \] (A.12)

Since \( \frac{\partial f}{\partial q_k} \geq \frac{\partial f}{\partial q_i} \) for \( i > k \), it is known that,

\[ \lambda_i = \frac{\partial f}{\partial q_k} - \frac{\partial f}{\partial q_i} \geq 0 \ (i = k + 1, \ldots, n) . \] (A.13)

Therefore, the Kuhn-Tucker conditions are satisfied.


Holland, J. (1975), Adaption in Natural and Artificial Systems, University of Michigan Press, Ann Arbor, MI.


Suarez-Soto, R.J., et al. (2008), Historical Reconstruction of PCE-Contaminated Drinking Water Using Probabilistic Analysis at U.S. Marine Corps Base Camp Lejeune, North Carolina, paper to be presented at World Environmental & Water Resources Congress, Honolulu, HI.


