

FINAL REPORT



NUMERICAL MODELING, RISK ASSESSMENT, AND SITE REMEDIATION

— A Study of Soil and Groundwater Contamination at the
Hoosier Gas Plant Site



Prepared by
Energy and Environment Program
Faculty of Engineering
University of Regina

Prepared for
Mr. Russell Roy, P.Eng.
Environmental Affairs
TransGas - SaskEnergy

August 1999

OUTLINE

1	Executive Summary
2	PART ONE Background
3	PART TWO Methodology for Subsurface Modeling
4	PART THREE Result of Subsurface Modeling
5	PART FOUR Risk Assessment
6	PART FIVE Design of Remediation Systems
7	PART SIX Conclusions
8	Appendices

EXECUTIVE SUMMARY

The Hoosier Gas Plant Site has been contaminated by benzene, toluene, ethyl-benzene, and xylenes (BTEX). Although a number of investigation projects have been undertaken, insight of site contamination, pollutant migration, biodegradation kinetics, and interactions among different phases is still unavailable. Many questions remain to be answered, such as:

- (1) What happen underground?
- (2) Are there specific impacts on the community?
- (3) What will happen in the future if we do not take any remediation action?
- (4) Which remediation technologies are suitable for the site?
- (5) What clean-up efficiency is needed?
- (6) When should we take actions?
- (7) Where should be the focus for the actions?

Answers to the above questions will help decision-makers to get insight into the current site situation. They will then know what they have to spend for, what they don't have to; how much they really have to spend, and how much is still uncertain. These will also be very helpful when they are discussing the problems (and the relevant decisions) with the local authorities.

A good decision will help to reduce a big amount of costs, while a not-so-good one may mean a number of consequences to the present and the future. For a complicated system, such as the site-contamination problem under consideration, this good decision should be based on good and thorough research efforts.

This project is to conduct a thorough study of the site to answer the above questions, according to the letter of September 19, 1997 from the Environmental Affairs, TransGas (see Appendix One). In detail, it consists of the following tasks:

- Modeling for the fate of petroleum contaminants in subsurface under various remediation scenarios,
- Environmental impact and risk assessments under various remediation scenarios,
- Recommended decisions for problem solving,
- Decision analysis for remediation actions,
- Operations analyses for monitoring networks (For Cantuar Field Site) (see Appendices Four to Six).

The results indicate that the above tasks have been successfully fulfilled.

The element of modeling for the fate of petroleum contaminants in subsurface is one of the most challenging tasks in this study. A large-scale numerical simulation model is developed for the site (Our program is the only organization in western Canada being also to conduct this type of simulation). The results are useful for:

- quantitatively answering questions related to site contamination situations under various remediation scenarios;
- predicting spatial distribution of contaminant concentrations in different time periods under each given remediation scenario;
- providing necessary inputs for further environmental impact and risk assessments.

The results of environmental impact and risk assessments are useful for:

- answering questions related to impacts and risks of the subsurface contamination under a variety of remediation scenarios;
- quantifying risks of different land use options under each given remediation scenario;
- identifying spatial distribution of risky zones and hot spots, required clean-up efficiency, and timing for remediation actions;
- providing necessary bases for decisions of remediation actions.

The task of remediation system design is undertaken based on analysis of site conditions, research of technology suitability, experimental studies for a number of remediation alternatives, as well as support of the earlier simulation and risk assessment tasks. The research outputs contain:

- recommendation for several remediation technologies that are feasible and applicable to the site;
- provision of detailed designs for the recommended remediation techniques;

This report consists of six parts. Part 1 is an introduction of the project and the study site. Part 2 details the methodology of numerical simulation for the fate of petroleum contaminants in subsurface. Part 3 illustrates formulation of the developed numerical model for the Hoosier Gas Plant Site, as well as modeling results for predicting concentrations of benzene, toluene, ethylbenzene, and xylenes in different temporal and spatial units under various remediation scenarios. Part 4 is to assess environmental risks of the subsurface contamination at the site, given different land use options, remediation scenarios, and evaluation criteria. Part 5 presents the results of remediation system design, where technologies that are feasible and applicable to the site are recommended, with the detailed designs provided. Part 6 is devoted to the summary of this project, which is followed by appendices.

TABLE OF CONTENTS

OUTLINE	1
EXECUTIVE SUMMARY	2
TABLE OF CONTENTS	4
PART ONE -- BACKGROUND	1
1. INTRODUCTION	2
2. SITE DESCRIPTION	8
2.1. Site Conditions	8
2.2. Site Contamination	17
2.3. Summary	19
PART TWO -- METHODOLOGY FOR SUBSURFACE MODELING	24
ABSTRACT	25
1. INTRODUCTION	26
2. LITERATURE REVIEW	27
2.1. FUNDAMENTALS OF LNAPL TRANSPORT THROUGH POROUS MEDIA	27
2.1.1 General Conceptual Model	27
2.1.2 Contaminant Phase Distribution	28
2.1.3 LNAPL Transport Parameters	28
2.1.4 LNAPL Migration at the Field Scale	32
2.2. FATE OF LNAPLs IN THE SUBSURFACE	34
2.2.1 Volatilization	34
2.2.2 Dissolution	35
2.2.3 Sorption	36

2.2.4	Biodegradation	37
2.3.	LNAPL IN GROUNDWATER SYSTEM	37
2.3.1	Mobile LNAPL	37
2.3.2	Apparent LNAPL Thickness	38
2.3.3	Apparent LNAPL Thickness Relationships	39
2.3.4	Soil Gas	40
2.3.5	Ground Water	40
2.4	LNAPL MODELING	41
2.4.1	Transport Processes	41
2.4.2	LNAPL Related Multiphase Flow Multi-Component Transport Modeling	45
2.4.3	LNAPL biodegradation modeling	46
2.4.4	Uncertainties Associated with LANPL Models	47
3.	ANALYSIS OF SINGLE PHASE FLOW	49
3.1.	DARCY'S LAW AND SINGLE WATER PHASE FLOW	49
3.1.1	Darcy's Law	49
3.1.2	Derivation of the Single Phase Flow Equation in A Porous Medium	49
3.2.	CONSTITUTIONAL RELATIONS AND SOLUTION METHOD	51
4.	ANALYSIS OF MULTI-PHASE FLOW MODELING	53
4.1.	GENERAL THREE-DIMENSIONAL THREE-PHASE FLOW EQUATIONS	53
4.2.	VERTICAL EQUILIBRIUM HEAD DISTRIBUTIONS	53
4.3.	VERTICAL INTEGRATION OF FLOW EQUATIONS	55
4.4.	CONSTITUTIVE RELATIONS	56
4.4.1	Two-phase Saturation-Pressure Relations	56
4.4.2	Extension to Three Phases	57
4.5.	ANALYSIS OF SATURATION DERIVES	58
4.6.	CHARACTERIZATION OF FLUID PERMEABILITY FUNCTIONS	59

4.7. VERTICALLY INTEGRATED SATURATION-PRESSURE RELATIONS	61
4.8. WATER AND OIL TRANSMISSIVITY RELATIONS	64
4.9. RESIDUAL NAPL VOLUME	66
4.9.1 Residual Oil due to Air-Oil Table Drawdown	66
4.9.2 Residual Oil due to Water Table Rising	66
4.10. INITIAL AND BOUNDARY CONDITIONS	67
4.10.1 Initial Conditions	67
4.10.2 Boundary conditions	67
4.10.3 Source/sink boundary condition	68
5. ANALYSIS OF NAPL MULTI-COMPONENT MODELING IN SUBSURFACE	69
5.1. DERIVATION OF THE GENERAL ADVECTION-DISPERSION EQUATION FOR MASS TRANSPORT IN FRACTURE MEDIA	69
5.2. MASS TRANSFER MODEL IN POROUS/FRACTURE MEDIA	70
5.3. ANALYSIS OF MULTI-PHASE MULTI-COMPONENT TRANSPORT	73
5.3.1 Equilibrium-controlled multi-phase transport	73
5.3.2 Transport with nonequilibrium inter-phase mass transfer	79
5.4. DECAY LOSSES IN THE MOBILE AND IMMOBILE PHASES (BIODEGRADATION)	82
5.4.1 Instantaneous reaction (Oxygen-limited)	82
5.4.2 Model Formulation for Aerobic and Anaerobic Degradation	84
5.4.3 Biodegradation of Daughter Products	86
5.5. LOADING FROM HYDROCARBON DISSOLUTION	87
5.6. ADDITIONAL INITIAL AND BOUNDARY CONDITIONS	87
6. SUMMARY	89
6.1. MODELING FORMULATION, SOLUTION, AND APPLICATION	89

6.2. CONSTITUTIONAL SUBMODELS FOR SOLUTION OF THE GOVERNING EQUATIONS OF MULTI-PHASE FLOW AND MULTI-COMPONENT TRANSPORT	90
6.2.1. Modeling system development and validation	90
6.2.2 Discussions of Nonhysteretic Multiphase Flow Modeling System	90
PART THREE -- RESULT OF SUBSURFACE MODELING	93
ABSTRACT	94
1. INTRODUCTION	96
2. MODELING FORMULATION	97
2.1. Single Phase Flow Model	97
2.2. Multi-Phase Flow Model	97
2.3. Multi-Component Transport Model	98
2.4. Biodegradation Model	99
2.5. Summary	100
3. MODELING SCHEMES	103
3.1. Conceptual Model	103
3.2. Simulation Scenarios	103
4. MODEL CONSTRUCTION	110
(1) Submodel of Groundwater Flow	110
(2) Submodel of Multi-Component Transport	111
5. DATA INVESTIGATION	112
6. MODEL EVALUATION AND TESTING	116
7. RESULTS	126
7.1. Simulation Outputs	126
(1) Scenario 1 (No Remediation Action is Undertaken)	126
(2) Scenario 2 (Remediation with 60% Efficiency)	144
(3) Scenario 3 (Remediation with 90% Efficiency)	158
7.2. Comparison and Discussion	171

(1) Site Contamination when no Remediation Action is Undertaken during 1998 to 2097	171
(2) Results along Three Lines when No Remediaton Action is Undertaken	176
(3) Simulation Results under Different Remediation Alternatives	190
7.3. Potential Impacts on Communities	196
8. DISCUSSIONS	197
9. SUMMARY	198
PART FOUR -- RISK ASSESSMENT	199
1. BACKGROUND	200
2. Methodology	202
2.1 Framework of Risk Assessment	202
2.2. Approaches for Risk Assessment	204
2.2.1. Multi-phase multi-component modeling	204
2.2.2. Assessment of risks caused by human exposure	206
2.2.3. Toxicity assessment	212
2.2.4. Risk characterization	217
3. RESULT ANALYSIS	218
3.1. Simulation Outputs for Risk Assessment	218
3.2. Risk Assessment for the Hoosier Site	227
3.3. Risk Assessment of Residential Land-Use Scenario	228
(A) <i>SERM-Based Risk Assessment</i>	228
3.3.1. SERM-Based Risk Assessment when No Remediation is Undertaken – [Scenario 1]	228
3.3.2. SERM-Based Risk Assessment under the 60% Remediation Scenario – [Scenario 2]	235

3.3.3. SERM-Based Risk Assessment under the 90% Remediation Scenario – [Scenario 3]	240
(B) <i>ELCR-Based Risk Assessment</i>	243
3.3.4. ELCR-Based Risk Assessment under the No-Remediation Scenario -- [Scenario 1]	243
3.3.5. ELCR-Based Risk Assessment under the 60% Remediation Scenario – [Scenario 2]	250
3.3.6. ELCR-Based Risk Assessment under a 90% Remediation Action – [Scenario 3]	252
3.4. Assessment of Risks when the Site is Used for Agricultural Activities (with Groundwater as Irrigation Water Resources)	257
3.4.1. SERM-Based Risk Assessment when No Remediation is Undertaken – [Scenario 1]	257
3.4.2. SERM-Based Risk Assessment under the 60% Remediation Scenario – [Scenario 2]	264
3.4.3. SERM-Based Risk Assessment under the 90% Remediation Scenario – [Scenario 3]	269
3.5. Risk Assessment when the Site is Used for Stockbreeding	271
3.6. Risk Assessment when the Land is Used for Fish Culture	272
3.7. Risk Assessment when the Land Remains as the Status Quo	273
3.7.1. SERM-Based Risk Assessment when No Remediation is Undertaken – [Scenario 1]	273
3.7.2. SERM-Based Risk Assessment under the 60% Remediation Scenario – [Scenario 2]	278
3.7.3. SERM-Based Risk Assessment under the 90% Remediation Scenario – [Scenario 3]	284
3.8. Assessment of Impacts on the Surrounding Communities	286
4. SUMMARY	287

PART FIVE -- DESIGN OF REMEDIATION SYSTEMS	288
ABSTRACT	289
1. INTRODUCTION	290
2. SCREENING OF REMEDIATION TECHNOLOGIES	291
2.1 Factors Affecting Selection of Remediation Technologies	291
2.2 Technology Screening Process	293
2.3 REMTEC Database	295
3. SITE INVESTIGATION	298
3.1 Stratigraphy	298
3.2 Groundwater	298
3.3 Site Contamination	298
3.3.1 Contamination sources	298
3.3.2 Contaminants	300
3.3.3 Free phase hydrocarbons	300
3.3.4 Residual phase and gaseous phase hydrocarbons	300
3.3.5 Dissolved Phase	300
4. APPLICABLE REMEDIATION TECHNOLOGIES	306
4.1 Site-Condition-Based Technology Selection	306
4.1.1. Applicable Technologies for the Contaminated Soil	306
4.1.2. Applicable Technologies for Contaminated Groundwater	306
4.2 Description of Potential Remediation Technologies	307
4.2.1. Landfarming	307
4.2.2. Low Temperature Thermal Desorption (LTTD)	309
4.2.3. Soil Vapor Extraction (SVE) and Pneumatic Fracturing Enhancement (PFE)	309
4.2.4. Air Sparging	312
4.2.5. In-Situ Bioremediation	314
5. PRELIMINARY REMEDIATION ALTERNATIVES	316
5.1 Hybrid Ex-Situ and In-Situ Remediation Alternatives	317

5.1.1.	Alternative 1: Excavation/Landfarming + In-Situ Bioremediation (LF + ISB)	317
5.1.2.	Alternative 2: Excavation/Landfarming + Soil Vapor Extraction + In-Situ Bioremediation (LF+SVE+ISB)	335
5.1.3.	Alternative 3: Excavation/Landfarming + Soil Vapor Extraction + Air Sparging + In-Situ Bioremediation (E-LF + SVE + AS + ISB)	345
5.1.4.	Alternative 4: Excavation/Low Temperature Thermal Desorption + In-Situ Bioremediation (LTTD + ISB)	353
5.2	Integrated In-Situ Remediation Alternatives	362
5.2.1.	Alternative 5: No-Excavation/In-Situ Bioremediation (ISB)	362
5.2.2.	Alternative 6: No-Excavation/Soil Vapor Extraction + Air Sparging + Pneumatic Fracturing Enhancement + In-situ bioremediation (SVE + AS + PFE + ISB)	364
6.	SUMMARY	371
PART SIX -- CONCLUSIONS		372
REFERENCES		373
APPENDICES		
Appendix One:	Letter of September 19, 1997 from the Environmental Affairs, TransGas (RE: Faculty of Engineering Research Proposal)	
Appendix Two:	Progress Report (Submitted on December 10, 1997)	
Appendix Three:	Letter to Russell Roy on December 16, 1998 (RE: Submission of Four Interim Reports)	
Appendix Four:	Design of a Monitoring Network for Detecting Underground Contamination — A Study for the Cantuar Field Site (SW 30-16- 16 W3M)	
Appendix Five:	Design of the Phase III Monitoring Program for the Cantuar Field Site (SW 30-16-16 W3M)	
Appendix Six:	Design for the Phase IV monitoring wells at the Cantuar Field Site (SW 30-16-16 W3M)	