Final Report, Contract B-239648

***Optimal Groundwater Remediation Design:
Methodologies and Software for Contaminated Aquifers***

Submitted to Lawrence Livermore National Laboratory

Prepared by David E. Dougherty, Principal Investigator

31 October 1994

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FINAL REPORT, CONTRACT B-239648
Optimal Groundwater Remediation
Design:
Methodologies and Software
for Contaminated Aquifers

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1. Executive Summary

This document comprises the final report of work performed under sub-contract B-239648 between the Lawrence Livermore National Laboratory (LLNL) and the University of Vermont (UVM). This contract was subsidiary to one between LLNL and the U. S. Department of Energy (DOE).

This project had the goal of developing tools and strategies to help make decisions regarding how and where and when to apply the environmental restoration (ER) technologies that are under development. The development of decision support software for advanced environmental remediation technologies is tentative; many of the ER technologies are poorly understood, the applicability of methods to new untested sites is questionable, the ability to predict the effects of alternative remediation designs is very limited, and there are a large number of uncertainties associated with processes and parameters (physical, chemical, and biological), contaminants (distribution and type), and sociopolitical environment. Nevertheless, the potential for significant savings by using optimal design methods and the need to make decisions regardless of uncertainties has made this project worthy.

This contract was active over the period of 24 June 1993 to 31 October 1994. An initial allocation of \$160,000 from LLNL to UVM was exhausted. This amount comprised about one fourth of the \$600,000 total project cost indicated in contract documents. A stop-work order was received in September 1994. An additional upper limit of \$15,000 was provided for project termination activities, including report preparation.

One of four deliverables was completed and provided to LLNL. MODLP is a computational tool for use in groundwater remediation design. It is a FORTRAN program that incorporates the well known and widely used MODFLOW simulator to represent flow of water in a saturated natural porous medium. MODLP is designed to allow the user to create and solve optimization problems for hydraulic control in groundwater systems.

Progress was made toward other deliverables. A moderate amount of work remains on one deliverable (regarding optimal design for solute removal), while significant work remains to be done on the other two deliverables. Two prototype pieces of software are provided in the final report; they are not suitable for distribution, yet represent some initiatives toward project completion that may be of interest.

Significant outreach efforts were made for a project with such a short effective lifetime. These include contacts within the DOE complex for potential applications and collaborations, presentations to DOE personnel and contractors, and presentations to the general engineering community.

Inasmuch as environmental restoration costs are very large, savings of on the order of ten percent represent significant amounts, and optimal design has been demonstrated to help produce savings larger than ten percent, these activities have an important role to play within DOE.

2. Introduction

2.1 Purpose and Organization

This document comprises the final report of work performed under sub-contract B-239648 between the Lawrence Livermore National Laboratory (LLNL) and the University of Vermont (UVM). This contract was subsidiary to one between LLNL and the U. S. Department of Energy (DOE).

This contract was active over the period of 24 June 1993 to 31 October 1994. An initial allocation of \$160,000 from LLNL to UVM was exhausted. This amount comprised about one fourth of the \$600,000 total project cost indicated in contract documents. A stop-work order was received in September 1994. An additional upper limit of \$15,000 was provided for project termination activities, including report preparation.

This work elements of this project are enumerated below, based on the Technical Task Proposal (TTP) between LLNL and DOE for Federal Fiscal Year 1993. These form the basis for the report format used.

1. Task 1: Optimal Design for Three-Dimensional Aquifers Using Hydrodynamic Constraints
2. Task 2: Optimal Design for Three-Dimensional Aquifers Including Solute Transport
3. Task 3: Optimal Design for Three-Dimensional Unsaturated Zone
4. Task 4: Improved Economic Realism
5. Task 5: User-Friendly Interfaces to Optimization Tools

This report then discusses efforts under the category of "Outreach and Technology Transfer". Following that are a summary, conclusions, and forward-looking remarks on advancing this work.

An alternative outline, based on the deliverables within the executed sub-contract, was not used so as to simplify final presentation of the project.

2.2 Technology Needs and Approach

Groundwater and soil contamination represent enormous environmental liabilities. Significant resources are being invested to develop and apply environmental remediation (ER) techniques to these problems. The U. S. Department of Energy's In Situ Remediation Integrated Demonstration Program, which funded this project, plays a very active role in this area.

Wise application of ER technologies requires (1) that the technology be appropriate to the type of contaminants and the risks associated with each, and (2) that the technology be applied in a cost-effective manner. It is, in other words, important to maximize risk reduction and to minimize cost, simultaneously.

This project had the goal of developing tools and strategies to help make decisions regarding how and where and when to apply the ER technologies that are under development. The development of decision support software for advanced environmental remediation technologies is tentative; many of the ER technologies are poorly understood, the applicability of methods to new untested sites is questionable, the ability to predict the effects of alternative remediation designs is very limited, and there are a large number of uncertainties associated with processes and parameters (physical, chemical, and biological), contaminants (distribution and type), and sociopolitical environment (de facto and de jure). Nevertheless, the potential for significant savings by using optimal design methods and the need to make decisions regardless of uncertainties has made this project worthy. These tools and strategies were the objectives of this project.

In brief, the approach is to (1) identify the key objectives, e.g. costs, in the ER design process for a particular ER technology at a particular site, (2) capture these dominant objectives mathematically in an objective function, (3) identify constraints that the design should satisfy including all physical processes and principals that apply (e.g., mass balance), (4) express the constraints in mathematical form including, for example, groundwater flow and transport models, and (5) solve the optimization problem given by the

objective function and the complete set of constraints.

Currently, it is infeasible to use a comprehensive representation of ER costs (see, for example, RACER [U. S. Air Force, 1994]). Instead, a cost model is used to assess those costs that most affect the design decisions.

Rigorous incorporation of uncertainty in design optimization for three-dimensional groundwater systems, saturated or unsaturated, has not been performed anywhere. Although ultimately vital to an effective decision support system, uncertainty is ignored in this project and processes are assumed to be deterministic.

This project is not a "modeling project", an oft-used pejorative in many geoenvironmental circles. Although mathematical and computational models of costs, constraints, and physical processes are required, the key aspect of this project is the identification and development of optimization tools for ER design. Particular ER technologies have been selected one-by-one to provide a practically oriented set of tools.

The sequence of tasks developed for this project are consistent with a progressive increase in problem difficulty and with the ER technologies deployed across the country. For saturated contaminated aquifers, hydrodynamic control is very widely used. Design based on actually cleaning up the contaminated region, rather than simply containing its spread, is also employed. These are the foci of Task 1 and Task 2, described below. In cases of contamination in the unsaturated zone, a variety of ER methods are being tested. One widely used one, soil vapor extraction, is usually design in the same way (with small changes for gas flow physics) as for hydrodynamic control of saturated aquifers [Sacks et al., 1994]. Many other ER techniques are being explored and developed. Task 3 is designed to address these unsaturated zone issues.

The optimization approach is effective when the economic model employed is sufficiently realistic to develop significant solutions. In recent years the cost models (as well as the process simulations and constraints) used in optimization problems have become more complex. This has led to increasingly difficult optimization problems and a need for new optimization tools. Task 4 addresses the need for increased realism in the economic models being used.

Finally, this work will have practical significance only if the tools are reason-

ably accessible for those acting as technical assistants or advisors to decision makers. User interface can play a substantial role in attracting staff to use more complex and comprehensive approaches, including those represented in this project. Task 5 focuses on improving such computer interfaces.

3. Task 1: Optimal Design for Three-Dimensional Aquifers Using Hydrodynamic Constraints

This task comprised the initial focus of work. The deliverable for this task was delivered to LLNL in December 1993 in the form of a computer program called MODLP and a User Guide.

When groundwater is found to be contaminated, one of the first impulses is to control the movement of the groundwater so that no contaminated water moves into undesirable regions. Upon further reflection, it is often desirable to restate the problem in terms of requiring groundwater flows to satisfy certain constraints at a variety of physical locations. In neither case are the contaminant concentrations themselves or masses directly constrained. Rather, the contaminants are assumed to travel in the porous medium, possibly with retardation and without dispersion. In saturated, confined, isothermal groundwater systems, the equations of groundwater flow are linear. As a result, the hydrodynamic constraints identified above are also linear. This fully linear case can be analyzed using a combination of a groundwater simulation model and a linear programming routine.

This approach, in which groundwater head and velocity are controlled as surrogates for concentration, is called the *hydrodynamic control*, or hydraulic capture, approach to remediation. This approach is widely used, almost always in two spatial dimensions [Gorelick et al., 1992].

The first deliverable in this project was a three-dimensional groundwater flow simulator coupled with a linear optimization solution procedure. The groundwater flow simulator selected was MODFLOW [MacDonald and Harbaugh,

1984]. The linear programming (LP) method called simplex was selected as the linear optimization routine. The resulting combination, named MODLP, retains the modular structure of the MODFLOW program and can be used with a calibrated model developed without consideration of hydrodynamic control. Thus, it is a product that can be layered on top of other modeling efforts to provide optimal design. To repeat, this optimal design is developed using (approximations of) the piezometric head and its gradients. It may, therefore, be viewed as the first-order approach to groundwater cleanup designs.

A technical description of the MODLP occupies the next several paragraphs. The User's Guide developed for this project is included as Appendix D of this report and a diskette containing the program comprises Appendix A.

3.1 Problem Description

Consider the following question, which comprises the hydrodynamic constraint problem. Given a groundwater simulator, a set of locations at which pumping wells can be located, and a list of the rates at which they may operate, choose which wells should be operated and with what intensity (extraction or injection rates) so as to minimize a cost and satisfy constraints on heads and gradients.

Let the total cost is the sum of fixed cost and operating-and-maintenance costs. To ensure a linear optimization problem will result, the latter are taken to be proportional to the rate of pumping from each well. That is, the decisional costs (total cost minus fixed cost) are associated with pumping and assumed to take a linear form such as

$$COST = \sum_{\text{wells}} C_{O\&M} Q_{\text{well}} , \quad (3.1)$$

where $C_{O\&M}$ is the cost of operation and maintenance per unit pumping rate Q_{well} at each well.

In practice, it is common to assume the hydrodynamic response of importance is the steady state groundwater flow system that usually develops a short time (relative to cleanup durations) after hydrodynamic control is instituted. The

constraints are assumed to be imposed at a single instant in time, at a variety of spatial locations.

In mathematical terms, we begin with a given three-dimensional, steady-state, saturated, isothermal groundwater flow system described by

$$S \frac{\partial h}{\partial t} - \nabla \cdot (K \cdot \nabla h) = q \quad (3.2)$$

and a given linear optimization problem (linear in both objective and constraints in terms of the head h)

$$\begin{aligned} &\text{Minimize } COST \\ &\text{subject to} \\ &Ah \leq a \text{ (heads)} \\ &B\nabla h \leq b \text{ (fluxes)} \\ &\text{Equation (3.2) (mass balance)} \end{aligned} \quad (3.3)$$

The problem is to find a set of pumping rates, at the prescribed potential well locations and with prescribed lower and upper bounds on pumping rates, that will minimize cost and satisfy all of the constraints.

3.2 Introduction to MODLP

MODLP is a computational tool for use in groundwater remediation design. It is a FORTRAN program that incorporates the well known and widely used MODFLOW simulator to represent flow of water in a saturated natural porous medium. MODLP is designed to allow the user to create and solve optimization problems for hydraulic control in groundwater systems. This is accomplished by coupling the groundwater flow simulation MODFLOW with a linear programming (LP) optimization solver.

Solving optimization problems involves two steps. First, the simulator is designed and calibrated to match the conditions in the system under study, using available data. The simulator is expected to provide an acceptable representation of the response of the field system to alternate pumping strategies. Second, LP optimization is used to solve for the set of pumping rates and locations that minimizes the weighted sum of pumping while simultaneously satisfying a number of user-specified constraints.

A description of MODFLOW [MacDonald and Harbaugh, 1984] or of its use is far beyond the scope of this document. Tersely, MODFLOW is a three-dimensional, transient or steady-state, saturated groundwater flow simulator developed by the U. S. Geological Survey. It may incorporate a single water table and a variety of commonly encountered, linear boundary and source conditions. The MODFLOW model does not represent solute transport, although it has been extended in a number of proprietary commercial codes to do so.

Users of MODLP are assumed to be familiar (and reasonably comfortable) with simulating groundwater flow using MODFLOW. The theory, limitations, and application of MODFLOW to groundwater flow problems will be assumed in this discussion. Information on these topics can be found in the User's Manual for MODFLOW [MacDonald and Harbaugh, 1984] and in the Tutorial Materials [Andersen, 1993] sponsored by the Environmental Protection Agency.

MODLP provides a "wrapper" around MODFLOW so that a calibrated groundwater flow model may be interrogated to assess the least cost solution to a groundwater cleanup problem that depends linearly upon the decisions to be taken and for which a set of constraints exist that are linear in the decisions. In its current form, MODLP accommodates vertical or horizontal injection or extraction wells (the wellbore physics are extremely simplified). It is applicable only to confined and leaky aquifer problems. (Phreatic surface problems are nonlinear and can be treated using the LP method only to the extent that they can be effectively modeled as if they were confined.)

Specification of the optimization problem requires that the user perform several steps:

1. A set of numerical discretization nodes to be considered as candidates for remediation pumping are selected.
2. The unit costs for injection and extraction pumping at each candidate well are specified.
3. Requirements on the hydraulic behavior of the groundwater system during remediation are selected from a set of possible constraints on head and pumping rates.

3.3 Coupling LP with MODFLOW

As previously mentioned, it is assumed that the user of MODLP has already constructed, calibrated, and verified a site-specific model of groundwater flow. To successfully couple this model with a linear optimizer, the MODFLOW simulations must be restricted. The MODFLOW model may contain any of the features of MODFLOW with the following exceptions:

1. The model must contain one stress period (i.e., NPER=1 in MODFLOW parlance).
2. The model must run to steady state (i.e., ISS=1 in MODFLOW).
3. The model must be of the constant transmissivity type (i.e., in MODFLOW set LAYCON=0 for all layers).

The first two exceptions are to maintain computational tractability, while the third is to maintain the linear response of head required by the linear programming formulation.

MODLP contains a complete copy of MODFLOW embedded within it. Only the main program unit, or driver, of MODFLOW has been modified so that it can be invoked repeatedly by the optimization routine. Therefore, a practical application of MODLP follows the construction and calibration of a MODFLOW model.

Once an acceptable design-worthy MODFLOW model has been completed, its input files can be used directly by MODLP without modification. A separate input file specific to MODLP must be created to describe the optimization problem. Note, however, that the MODFLOW input data files are not at all affected by use of MODLP, so they can be preserved for archival and recalibration purposes.

3.4 Constraints and Objective Functions in MODLP

The optimization portion of MODLP always seeks the pumping strategy with the least "cost" associated with it. This cost is defined by the user by placing units costs for injection and extraction pumping at each candidate pumping well. The total cost that is minimized is measured as the sum of the products

of the unit costs at each well and the flow rate at the well. Mathematically, the objective function is represented by the weighted sum of withdrawal and recharge rates as

$$\Phi = \sum_{\text{wells}} q_j^+ \beta_j + \sum_{\text{wells}} q_j^- \beta_j^-, \quad (3.4)$$

where j is the relative cost coefficient that related the rate of pumping to the cost of pumping at location j . Note that if injection or extraction are considered at a single spatial location, then there are two decision variables (and two terms in the objective function) corresponding to that one point in space. The use of this cost function presumes that the cost of operation of the hydraulic control system is linearly proportional to the rate of pumping.

Input requirements for each of these constraint types are described below. MODLP can define two types of constraints on the hydraulic head and one kind of constraint on the pumping rates.

1. An absolute bound may be placed on heads at a point:

$$h_i \geq h_{i,l}^* \quad (3.5)$$

or

$$h_i \leq h_{i,u}^* \quad (3.6)$$

where $h_{i,l}^*$ and $h_{i,u}^*$ are specified lower and upper values and h_i is the head at a node where control is to be imposed. Depending on the direction of the inequality, the type of constraint can be used to control excessive drawdown (3.5) or mounding (3.6) of the piezometric surface.

2. Requirements may be placed on the difference in heads:

$$h_{i1} - h_{i2} \geq d_i^* \quad (3.7)$$

where d_i^* is the specified bound on head differences, and h_{i1} and h_{i2} are the heads at (often adjoining) node points i_1 and i_2 , respectively. This constraint can be used to force a gradient in the hydraulic flow field, either horizontally or vertically.

3. Constraints commonly are placed on withdrawal and recharge rates to express bounds on well yield or limitations on the rate at which water can be recharged. Bounds can be imposed on flux rates, either withdrawal or recharge, as follows where q_j is an individual flux rate at location j and q_{jmax} is the maximum recharge or withdrawal rate respectively that can be achieved at location j .

4. Task 2: Optimal Design for Three-Dimensional Aquifers Including Solute Transport

Work began on this task in the summer of 1993. This task was not completed as a result of insufficient funds. At the time that funds were exhausted, approximately 60% of the subtasks identified for this task were completed.

The next more sophisticated approach to optimal design for contaminated groundwater systems incorporates the amount by which concentrations or total mass of contaminant are reduced due to cleanup activities. This contrasts with the hydrodynamic approach of Chapter 3, which focuses on containment of groundwater flows within a specified region. The optimal cleanup problem is more difficult than the optimal containment problem. In the former the concentrations are nonlinearly dependent on design decision variables, whereas the heads and gradients are linearly related to pump-and-treat decision variables in the capture-zone problem. Thus, nonlinear optimization is required.

The technical nature of the nonlinear optimization, viz., whether the problem is convex or non-convex, is problem-specific. As a result, design optimization methods identified or developed for this task need to be able to handle fairly general nonlinear situations and yet be practical.

4.1 Approach

The approach taken in this task was as follows.

1. Identify physical, chemical, biological, and remediation processes that needed to be considered.
2. Identify reasonable economic model for representing the cost of various remediation schemes.
3. Identify candidate optimization methods suitable to the task of optimizing given the results of steps 1 and 2.
4. Test candidate optimization methods with realistic two-dimensional site-specific groundwater flow and solute transport model(s).
5. Possibly in parallel with steps 3 and 4, identify candidate three-dimensional models for inclusion in the deliverable for this task.
6. Select a three-dimensional model for inclusion in the task deliverable.
7. Combine model with optimization method(s).
8. Test combined optimizer-simulator(s).
9. Select combined optimizer-simulator for deliverable.

4.2 Identifying the Processes to be Included

The processes to be included under this task were, in fact, identified in the proposal from the University of Vermont to LLNL. These are the processes commonly included in isothermal, single phase, solute transport models with adsorption, relatively low concentrations (implying no affect on fluid density by contaminant concentration), and no biological activity. Inclusion of biological terms was considered important; however, they were considered something that could be incorporated after the first order processes were accommodated. Initially work would be associated with pump-and-treat technologies.

4.3 Identifying the Economic Model to be Included

Again, the proposal was fairly specific about costs that should be included. These are costs that depend on the amount of water pumped, the amount of water treated, the amount of water injected, and the amount of time the

remediation system is in operation. Including the number of wells installed as an indicator of costs is an element of the "enhanced economic realism" task reported later in this document.

Thus, the initial cost model had the elements

- Cost of pumping
- Cost of treatment
- Cost of injection
- Cost of operation and maintenance.

See Chapter 7 of this report.

4.4 Identifying the Simulator to be Included

In the summer of 1993, shortly after this subcontract was signed, an informal survey of groundwater modelers and publications associated with Integrated Demonstrations, DOE-lab CERCLA activities, and other Department of Energy initiatives was conducted. The purpose of this activity was to identify one or more widely used three-dimensional models of solute transport in water-saturated groundwater systems. The intent of this survey was to identify a small number of candidate groundwater codes that would be considered for the analysis "engine" that would be coupled with an optimizer.

As communicated in monthly reports earlier in the project, the results of this survey were inconclusive. Apparently, each group that uses groundwater models makes an independent assessment of its needs and expertise. As a result there seems to be no generic groundwater model that is suitable for all sites, is uniformly well known, and/or embodies the physical, chemical, biological, and remediation processes deemed necessary for site-specific application. A "not invented here" syndrome was perceived among some modelers as well.

As a result of this informal survey, a well known and widely available solute transport computer program called MT3D [Papadopoulos and Associates, 1992] was selected for this task. MT3D has been successfully compiled on run on machines ranging from a DOS-based personal computer to a Cray.

A fractional employee was given responsibility for becoming knowledgeable of MT3D so that it could be integrated with the optimization methods that would be identified, tested, or possibly developed.

4.5 Identifying the Optimizer to be Included

In the summer of 1993, shortly after this subcontract was signed, informal tests of the outer approximation method were conducted. This method of optimization has been in research and development for geohydrological applications by Karatzas and Pinder [1993]. These tests focused on scaling issues (how does the method perform as the problem size increases) and dimensional issues (how does the method perform on three-dimensional problems) for the saturated zone. The results of this investigation were satisfying. In three-dimensional saturated zone solute transport problems, the method performed quite well and its behavior was similar in major respects to two-dimensional problems. Scaling is a difficult issue in all optimization methods for nonlinear problems. The outer approximation method appears to scale very well, especially when compared to traditional nonlinear optimization packages such as MINOS (see [Gorelick et al., 1988]), which has been used many times in geohydrological applications. Figure 4.1 from Karatzas et al. [1994] suggests the relative performance of a variant of the outer approximation and MINOS optimization methods.

Preliminary tests of the outer approximation method were conducted for pump-and-treat remediation using fixed costs proportional to the number of wells installed and operating costs proportional to the pumping rate selected. These tests were performed before the selection of MT3D and using proprietary computer codes. Results indicated that the outer approximation method offers a good opportunity for development of a method appropriate for this project.

Figure 4.1: Computational effort versus problem size for variant of outer approximation method and for MINOS (after Karatzas et al. [1994]).

5. Task 3: Optimal Design for Three-Dimensional Unsaturated Zone

Work began on this large task in the late spring of 1994. This task was not completed as a result of insufficient funds. Work was initiated on 3 of 10 identified subtasks.

Contamination within the unsaturated zone, which is the region between the ground surface and the water table of a subsurface aquifer, often acts as a long-term source of contaminant to the underlying aquifer. Therefore, controlling and remediating unsaturated zone contamination is a form of source control, at least with respect to the saturated groundwater system.

Unsaturated zone remediation is being vigorously pursued across the United States and Europe. The most common problem being tackled is petroleum-based or -related chemicals, including components of gasoline, fuel oil, and heating oil. Often the chemical contaminants are identified by BTEX (benzene, toluene, ethyl benzene, and xylene), although many other compounds with higher molecular weights are also present. Volatile organic compounds (VOCs) comprise another group of widely encountered contaminants. Many of the common ones are halogenated aliphatics.

The BTEX components and VOCs are volatile, so methods based on in situ air stripping (including soil vapor extraction, soil venting, and other perturbations on the technology) are widely used. Sometimes it is combined with enhancement methods such as heating.

The low molecular weight aromatic components of the petroleum products are also susceptible to the aerobic action of many naturally occurring microorganisms, which produce enzymes that lead to the elimination of carbon rings and the eventual conversion of the compound to water, carbon dioxide, and other innocuous by-products. The chlorinated aliphatic hydrocarbons (CAHs), such as carbon tetrachloride (CT) and trichloroethene (TCE), can be dehalogenated under anaerobic conditions by cometabolism. In principal, anaerobic transformation of CAHs can result in innocuous byproducts (CO_2 , H_2O , and Cl^-). However, according to McCarty and Semprini [1994], (1) a primary organic compound must be present for cometabolism, (2) transformation rates are slow, (3) some intermediate transformation products are more hazardous than the parent compounds, (4) reaction rates are highest under methane-producing, highly reducing environments, and (5) the microorganisms that can bring about the cometabolic transformations must be present.

There are high molecular weight compounds in petroleum products, such as creosote, that are much less susceptible to biological decomposition or volatilization-based processes. For these compounds a different set of microorganisms and microenvironments are being investigated (also for use with high molecular weight compounds such as the polycyclic aromatic hydrocarbons, or PAHs, and polychlorinated benzenes, or PCBs). Combinations of treatments, e.g., anaerobic transformation followed by aerobic bioremediation, may prove appropriate to such challenges [McCarty and Semprini, 1994]. Other destructive biological methods are also being investigated in groups across the country. The monograph produced by the National Research Council [1993] provides a current overview of this technology.

Many other environmental remediation technologies being arrayed against unsaturated zone contamination. Among them are soil heating, soil washing, solvent-extraction, in situ vitrification, excavation, air sparging, and engineered barrier systems. Example projects within the DOE's In Situ Remediation Integrated Demonstration Program are listed in Table 5.1.

Optimal design for contaminated unsaturated-zone groundwater systems must incorporate the physics and mechanisms of flow in the unsaturated zone, which are highly nonlinear. In addition, those processes that are dominant factors in the remediation technologies must be included within the process

Project Title	Project Description
Chemically Enhanced Barriers to Minimize Contaminant Migration	Chemical barriers to contaminant movement in unsaturated zone, including adsorption, reduction, precipitation, and sequestration.
Containment of Contaminants Through Physical Barriers Formed from Viscous Liquids Emplaced Under Controlled Viscosity Conditions	Plumes trapped and immobilized by injected fluid barriers that are nearly inert and impermeable
Evaluation of Two New Flowable Grout Techniques	Grout barriers comprising bentonite-mineral wax and proprietary inorganic grout
Hydraulic and Diffusion Barriers in the Vadose Zone Surrounding Buried Waste	Testing and developing new barrier materials for buried waste control
Demonstration of a Frozen Soil Barrier at an Arid Site	Feasibility of containing vadose zone contaminants using ground freezing
Surface Controlled Emplacement of Horizontal Barriers Beneath Waste Sites	Grouting through horizontal drill holes constructed under contaminant region
In Situ Corona for In Situ Treatment of Non-Volatile Organic Contaminants	Gas-phase oxidants are created by a strong electric field generated in the subsurface
In Situ Chemical Treatment	Feasibility of treating soils by injecting reactive gases
Field Demonstration of Electrokinetic Migration Technology at Old TNX Basin	Electrokinetic migration of mercury contaminated unsaturated soils
Electrokinetic Remediation of Heavy Metal Contaminated Unsaturated Soil	Electrokinetic migration in chromate contaminated unsaturated soils
In Situ Remediation by Electrokinetics	Electrokinetic migration of uranium contaminated unsaturated soils

Table 5.1: Example technology projects within the DOE In Situ Remediation Integrated Demonstration Program pertaining to unsaturated zone remediation or containment (after U. S. Department of Energy [1994]).

simulator that forms the core of the optimal design approach. The latter processes may be very nonlinear (a technology exemplifying this is electrokinetic migration). Thus, there will be nonlinear flow, nonlinear transport, and nonlinear reactions occurring simultaneously. Clearly, this problem is more complex than either hydrodynamic containment or pump-and-treat cleanup methods for saturated aquifers discussed earlier in this report. Nonlinear optimization is required, and it may well be much more difficult than for remediation of the saturated zone.

The technical nature of the nonlinear optimization, viz. whether the problem is convex or non-convex, is problem-specific. As a result, design optimization methods identified or developed for this task need to be able to handle fairly general nonlinear situations and yet be practical.

5.1 Approach

The approach initiated for this task was as follows.

1. Identify physical, chemical, biological, and remediation processes that needed to be considered.
2. Identify reasonable economic model for representing the cost of various remediation schemes.
3. Identify candidate optimization methods suitable to the task of optimizing given the results of steps 1 and 2.
4. Test candidate optimization methods with realistic two-dimensional site-specific unsaturated-zone simulation model(s).
5. Possibly in parallel with steps 3 and 4, identify candidate three-dimensional models for inclusion in the deliverable for this task.
6. Select a three-dimensional simulator for inclusion in the task deliverable.
7. Combine simulator with optimization methods.
8. Test combined optimizer-simulator.
9. Select combined optimizer-simulator for deliverable.

10. Add elements to user interface for unsaturated zone scenarios.

5.2 Identifying the Processes to be Included

The processes to be included under this task were partially identified above and in the proposal from the University of Vermont to LLNL. However, a manageable project requires that a more limited range of options be considered within this project. Indeed, many of the processes indicated earlier in this section are not fully understood and cannot be simulated accurately.

At the time that project funds were exhausted, a post-doctoral research associate was focusing on this issue. The technologies receiving most attention when work stopped were (1) soil vapor extraction, (2) soil venting, (3) dry heating (not steam injection), and (4) in situ bioremediation.

5.3 Identifying the Economic Model to be Included

The components of the economic model could not be identified until the remediation process(es) of interest were identified. A literature review of Department of Energy-funded research on the economics of various remediation technologies was begun (e.g., Schroeder et al. [1992]). Inasmuch as the remediation process(es) and simulator(s) had not been identified at the effective end of this project (June 1994), this task was not advanced.

5.4 Identifying the Simulator to be Included

In the summer of 1993, shortly after this subcontract was signed, an informal survey of groundwater modelers and publications associated with Integrated Demonstrations, DOE-lab CERCLA activities, and other Department of Energy initiatives was conducted. The purpose of this activity was to identify one or more widely used three dimensional models of solute transport in water-saturated groundwater systems. The intent of this survey was to identify a small number of candidate groundwater codes that would be considered for the analysis "engine".

As communicated in monthly reports earlier in the project, the results of this survey were inconclusive. Apparently, each group that uses unsaturated

groundwater models makes an independent assessment of its needs and expertise. As a result there seems to be no generic groundwater model that is suitable for all sites, is uniformly well known, and/or embodies the physical, chemical, biological, and remediation processes deemed necessary for site-specific application. A "not invented here" syndrome was perceived among some modelers as well.

A report examining the capabilities of numerous unsaturated zone models, with particular reference to application at the Yucca Mountain Project, was reviewed [Intera, 1993]. Eighteen major models were evaluated including eight fully three-dimensional ones. These codes are typically multiphase fluid flow codes, hence computationally intensive, rather than single-phase models based on Richards equation.

During the short time this task was active, no three dimensional, multiphase fluid flow model was identified with an adequate representation of the bioremediation process.

No single simulator was selected by the end of the active lifetime of this project.

5.5 Identifying the Optimizer to be Included

The method of optimization for the unsaturated case was not selected. This would occur after the optimization for saturated solute-transport problems was settled, as the latter is also applied to a nonlinear problem, and after the unsaturated zone processes were established. The number of candidate methods for the optimization technique is relatively small, and grows if only a small number of design decisions require optimization. Among candidates are "traditional" nonlinear programming methods (e.g., MINOS), approximation methods (e.g., outer approximation method), and heuristic methods (e.g., genetic algorithms). Again, work stopped on this project before a selection was made among alternatives.

6. Task 4: Improved Economic Realism

6.1 Cost Models and Cost Estimates

In addition to simulation tools, an effective optimal design system requires reasonably realistic *cost* (or benefit) *models*. It should be clearly seen that the economic or cost model used in a design optimization setting is not a true project cost estimate. Just as a mathematical model can be used during design as a surrogate for the real process of interest, so too is a cost model a surrogate for a comprehensive cost estimate. The latter is usually quite complicated (though not complex) and, if used directly within the optimization approach, can lead to many very difficult mathematical problems (usually involving the mathematical issues of smoothness, differentiability, and well-posedness). The ENVEST software developed by the U. S. Air Force [U. S. Air Force, 1994] is a remarkable example of a comprehensive cost estimation package.

6.2 Elements of Cost Models

Traditionally in computer-aided groundwater design the cost is modeled quite simply. Usually, it has been expressed as a coefficient times the rate of pumping times the duration of pumping, assuming a pump-and-treat design is being considered. The coefficient may include present value factors, and treatment and disposal costs per unit volume pumped, for example.

Fixed costs have been included in a small number of papers but not in practice, because the resulting problem has led to computationally intractable difficulties when using the mixed integer programming approach. Recently, however, alternative optimization approaches allow fixed costs, especially a fixed cost proportional to the number of wells installed in a pump-and-treat system, to be included. Two such methods are the outer approximation method [Karatzas and Pinder, 1993] and the simulated annealing method [Dougherty and Marryott, 1991; Marryott et al., 1993].

Another significant cost element not represented completely by either of the previously mentioned cost terms is piping from wells to treatment plants and on to discharge points. A number of estimating methods (e.g., RACER [U. S. Air Force, 1994]) can associate a typical piping distance and per-length cost to each installed well. This approach is currently being used at LLNL [Leah Rogers, personal communication, 1994], UVM [Donna Rizzo, personal communication, 1994], and elsewhere.

A survey was begun in June 1994 to document the various cost models for aquifer (i.e., saturated zone) remediation that have been reported in the literature. Many sources of information, notably technical reports that are not cataloged by libraries, were not available with our searching procedures. A sampler of findings is presented in Table 6.2. A more extensive reference list is included in the bibliography of this report.

The preceding discussion clearly indicates that the trend in design optimization is to incorporate increasingly complex cost elements into cost models. The ability to include alternative remediation techniques and fixed costs into cost models is increasingly important. As the actual costs of ER become apparent, budgeting for ER is effectively a per annum total cost. This leads to a need for prioritization among sites according to risk, risk reduction per unit cost, etc. It also generates a need to reduce the remediation time as a significant to impact the total ER cost. Kuo et al. [1992] and Sacks et al. [1994] indicate this direction for saturated and unsaturated zone remediation, respectively.

As design optimization tools are turned to those most challenging of ER problems within the DOE complex, new cost elements can be anticipated. An example is the cost of competition in the remediation of multiple and mixed wastes. A second example is the cost of monitoring and evaluation associated with cleanup technologies and the intensity of their application. These cost elements are both extensions of current cost elements and expansions of perspective on the costs of ER.

Item #	Cost Elements	Reference
1	Treatment, $\propto Q$	Ahlfeld, 1990
2	Treatment, $\propto Q$	Ahlfeld and Sawyer, 1990
3	Expected value of: Mixed costs, $f(Q, h, c)$ Final costs, $g(h, c)$	Andricevic, 1990
4a	Installation, $\propto N_Q$ Treatment, $\propto Q$ Energy, $\propto Q^2$ Penalty, $f(Q, h)$	Dougherty and Marryott, 1991
4b	Installation, $\propto N_Q$ Treatment, $\propto Q$ Penalty, $f(c)$	Dougherty and Marryott, 1991
4c	Installation, $\propto N_Q$ Treatment, $\propto Q$ Penalty, $f(c)$ Cutoff wall, $\propto L_w$	Dougherty and Marryott, 1991
5	Treatment, $\propto Q$ Energy, $\propto Qh$ Penalty, $f(Q, c)$	Chang, Shoemaker, and Liu, 1992
6	Treatment, $\propto Q$ Energy, $\propto Qh$ Penalty, $f(c)$	Culver and Shoemaker, 1992
7a	Treatment, $\propto Q$	Gorelick et al., 1992
7b	Treatment periods, $\propto Q(t)$	Gorelick et al., 1992
8	Treatment, $\propto Q$ Cleanup time, $\propto t_c$ Penalty, $f(c)$	Kuo et al., 1992
9	Treatment, $\propto Q$ Energy, $\propto Qh$ Penalty, $f(c)$	Culver and Shoemaker, 1993
10	Treatment, $\propto Q$ Well Installation, $\propto 1 - e^{-bQ}$	Karatzas and Pinder, 1993
11	Treatment, $\propto Q$	Ahlfeld, 1994

Table 6.1: Some cost elements from recent literature sources. Q , well flow rates; L_w , cutoff wall length, t_c , time spent remediating; f and g , functions of their arguments; b , constant; h , head; c , concentration,

7. Task 5: User-Friendly Interfaces to Optimization Tools

This task was initiated in June 1993 and was conducted through June 1994. Initial work proceeded in parallel with other work. This task was not completed due to insufficient project funds. Progress toward deliverables is discussed below.

7.1 Approach

The approach initiated for this task was as follows.

1. Identify computer platforms that needed to be considered.
2. Identify types of functionality required for groundwater simulations.
3. Identify types of functionality required for decision-making use.
4. Identify alternative interface designs.
5. Identify alternative implementation strategies and test if necessary.
6. Select an implementation.
7. Develop interface components.
8. Test.

7.2 Computer Platforms

A wide variety of computer platforms are used within the DOE laboratories, DOE contractors, and environmental consultants. This provides a software engineering challenge of greater magnitude than desirable. DOS-based PCs, Windows-based PCs, Windows-NT based workstations, Macintoshes, and workstations from Data General, Digital, Hewlett-Packard, IBM, Silicon Graphics, Sun Microsystems, and others were found to be used in these communities.

To simplify our efforts and to be consistent with the approach we believe will be used in the practice, we avoided attaching the work to any specific hardware or operating system. Instead, software environments were considered that could be used on many different machines. Efficient use of computer resources was not a major factor in these decisions; the costs of computer resources is significantly less than the costs of a person sufficiently skilled to use the products of this project. (As examples, a Pentium PC (fully configured) costs on the order of \$5000 and a personal Unix-based workstation (similarly configured) costs on the order of \$10,000.)

7.3 Functionality Issues

Two important elements of any computer-based decision process are preprocessing and postprocessing of the decision-making analysis. Preprocessing includes, importantly, the embodiment of a problem's specification into the input dataset of the analysis processor. Once the processor has been invoked, postprocessing is used to display and interrogate the result of analysis.

Preprocessing is often performed using DOS-based programs written for a specific groundwater simulator. We have looked at methods that would not reproduce the existing packages. Instead we have operated under the view that groundwater simulation datasets will be developed in the way they have over the last several years. Where we are adding value and need to add pre-processing is in the specification of the optimization model, including the specification of the elements of the cost function and creation of datasets specifying each optimization problem.

Two efforts in this area were undertaken, one using Tcl/Tk [Ousterhout,

1994] for creating and modifying input datasets for MODLP (see Section 2.2), and a second using Matlab “uicontrols” [MathWorks, 1994] to provide graphically oriented input for unspecified optimization packages. This work was part of the “economic model” and of the “user interface for optimization tools”. These two efforts were experimental in nature; they do not accurately portray what might have resulted

As part of the informal survey mentioned above under Task 3, experts at a number of DOE-funded facilities were asked to describe the computer hardware and software used for post-processing of results. The results, like the results of the previously mentioned process modeling survey, indicate that there is not single software package that is used ubiquitously. Two possibly resulting scenarios come to mind. First, select a post-processing unilaterally and hope that others will find the choice was wise. A second approach is the one that was actually selected. Given that it is difficult to identify a consensus-based post-processing package, a workable solution is to write a well-documented file suitable for post-processing by the large number of packages used within the DOE community, that is write a “neutral file”.

7.4 Problem Description Interfaces

7.4.1 Tcl/Tk Interface for MODLP-Specific Dataset

As described earlier, MODLP has been constructed as a “wrapper” around the MODFLOW program. A single additional dataset is added to the MODFLOW data files to describe a MODLP problem. Because optimal design occurs using a groundwater flow model that has already been constructed and calibrated, and because there are a number of readily available and widely used “preprocessors” for MODFLOW (indeed a new program called “Visual MODFLOW” is now being beta tested by Waterloo Hydrogeologic Software), it was decided to develop a prototype of a user interface that could be used to build the MODLP-specific dataset was constructed.

The interface was built using a software package called Tcl/TK (“tickle tee kay”), which is available for a number of computers, including PCs, Macintoshes, and Unix workstations. Tck/Tk is basically an interface to the graphical intrinsics in X-windows or other graphics software systems. Applications built using Tcl/Tk are essentially interpreted, rather than compiled,

so the user interface developed for MODLP requires one to carry the Tcl/Tk software, as well as the interface application itself.

The MODLP interface prototype was called *xmodopt*. It uses a set of pull-down menu items and data entry forms to simplify the description of a specific hydrodynamic optimization problem.

Xmodopt was not extensively tested or used, as it was a prototype. The basic concept of *xmodopt* is believed to be solid. One area recognized as needing improvement is in describing the geometric location(s) of capture zone constraint location(s) in an intuitive way. In this initial attempt, we have resorted to a text based entry system.

It is important to reiterate that the Tcl/Tk-based *xmodopt* is a proof-of-concept piece of software only. It has not been tested in a production environment, and the software is minimally documented. *Xmodopt* is included on diskette in Appendix B to more fully describe the scope of the activities undertaken in this project.

⇒ We strongly discourage any distribution of this software.

7.4.2 Matlab-Based Interface for Describing Economic Model

When one uses an optimal design code, the optimization is driven by the objective function and by the set of constraints that must be satisfied. A prototype of an interface for entering such information was developed using Matlab, a widely available commercial software package [MathWorks, 1994] that requires a license. The prototype developed here is contained in a set of "M-files", which the Matlab package uses as "scripts". (Actually, it may be more convenient to view the M-files as source codes for Matlab, which partially compiles them during execution but does not create compiled stand-alone executables.)

The intent in this interface project was to develop a tool that could be used for describing a variety of optimization problems, and hence to provide the basis for the integrated interface for this subcontract. Simply named *optimizer*, this prototype has certain key features that are very attractive for the subcontract as it was envisaged.

1. It allows one of several different optimization methods to be selected

by a user with a click on a button. This selection provides a context for further information that a user would be required, allowed, or precluded from entry. For example, the use of a MINOS-based optimization does not allow fixed costs to be included in the problem description.

2. It provides an innovative way to enter the objective function. A user is confronted with a set of buttons, each labeled with a word in English, that may be clicked. As each button is clicked, a sentence fragment is formed that describes the objective. An example fragment would be "minimize pumping". Because multiple objectives are the norm in practical optimization, the grammar of this feature includes "and" and "or", as well as parentheses to demark meanings unambiguously. A weight can be set for each element of the objective function (often called utility coefficients, or some such name). Figure 7.1 shows this feature as it appears on the computer screen. Once the sentence has been constructed properly, the sentence is parsed and compiled, using the Unix utility *yacc* (which is also available for other non-Unix machines, such as the PC, from the Free Software Foundation).
3. This prototype has a help utility, which allows one to point at an option (button) on the screen and have a help window pop up. At the current point of development, this feature does not provide an extensive amount of assistance. The proof of concept is complete, however.
4. The optimizer can be launched from the *optimizer* tool, once the problem has been described. Alternatively, the problem description can be saved in a file for later use or revision. Versions are managed with project file names and with multiple scenarios within a given version of a problem.
5. Problem descriptions are saved in two important ways. First, the problem description can be saved in a format so that *optimizer* can reload the description for editing. Second, a particular scenario can be saved in data files appropriate for the optimization method selected within that scenario. These data files can then be used directly to launch the optimization programs outside of the *optimizer* tool.

It is important to reiterate that the Matlab-based *optimizer* is a proof-of-concept piece of software only. It has not been tested in a production envi-

ronment, and not all of its buttons and options have been connected together. (For example, pressing the “execute” button will not, at this time, actually launch an optimizer.) Nor is the software documented. It contains references to optimizers or optimization features that may not exist or may not be publicly available. *Optimizer* is included on diskette as Appendix C to more fully describe the scope of the activities undertaken in this project.

⇒ We strongly discourage any distribution of this software.

Cost Function

Maximize

Minimize

Construction

Treatment

Delete

Close

Constraints

Total Simulation Time (years)	30
Number Of Management Periods	1
Maximum Number Of Wells Installed Over Total Simulation Time	25
Maximum Number Of Wells Allowed To Pump During Any One Management Period	15
Contaminant Of Concern	TCE
State Or Federal Drinking Water Standard For TCE (ppb)	5
<div> ☒ <div>Base Well Location</div> </div>	

Apply

Done

Cancel

Figure 7.1: Sample of user interface provided in *optimizer*.

8. Outreach and Technology Transfer

Our commitment to outreach and technology transfer has been fulfilled energetically.

During the period spanning July 1993 (when the subcontract was in place) to July 1994 (when funds were depleted, except for final reporting), the following actions occurred.

1. October 1993, Participant in ER'93 in Augusta, GA
2. December 1993, MODLP released to LLNL
3. January 1994, Poster at DOE EM-40/EM-50 meeting in Seattle, WA
4. February 1994, Participants in ISRIP PI meeting in Houston, TX
5. July 1994, MODLP released for distribution to Argonne Code Library

Numerous informal exchanges and presentations were made throughout the year. Discussions were initiated with individuals at a number of DOE facilities to identify ways in which the results of this project could in future provide direct benefit to their responsibilities. Sites included Los Alamos, Savannah River, Hanford, and Livermore.

Publications and presentations at conferences were also derived from this project, in whole or in part, as listed below in chronological order.

1. D. E. Dougherty, "Finite Element Methods in Geoenvironmental Restoration", VIII International Conference on Finite Elements in Fluids, Universitat Polytechnica de Catalunya, Barcelona, Spain, September 1993.

2. D. P. Ahlfeld and D. E. Dougherty, "MODLP Program Description: A Program for Solving Linear Optimal Hydraulic Control of Groundwater Contamination Based on MODFLOW Simulation", Research Center for Groundwater Remediation Design, University of Vermont, Burlington, VT, 1993.
3. W. A. McGrath and G. F. Pinder, "Locating Contaminant Plumes Under Uncertainty", American Geophysical Union, Fall Meeting, San Francisco, December 1993.
4. D. W. Rice, J. P. Ziagos, and D. E. Dougherty, "Decision Support for Environmental Restoration", (Poster) Joint EM-40/EM-50 Industry Outreach Meeting, Department of Energy, Seattle, WA, January 1994.
5. D. E. Dougherty, "Building Groundwater Optimizers That Respond to the Needs of Decision-Makers", *Water Policy and Management: Solving the Problems*, Proceedings of the Annual Water Resources, Planning, and Management Conference, American Society of Civil Engineers, pp. 347-350, 1994.
6. W. A. McGrath and G. F. Pinder, "Delineating a Contaminant Plume Boundary", *Computational Methods in Water Resources X, Volume 1*, Kluwer Academic Press, pp. 317-324, 1994.

9. Summary and Conclusions

1. This subcontract, while officially active from the end of June 1993 to the end of October 1994, had a life of project activity from July 1993 to July 1994. The funding level made available to the University of Vermont from Lawrence Livermore National Laboratory, excluding costs of fulfilling the stop-work order from the Department of Energy, was \$160,000. This value represents the total costs, including all personnel benefits, indirect costs, and subcontract costs. This value represents about 27% of the total contract amount provided in the contract between LLNL and UVM.
2. During this twelve months, significant technical progress was made. One of the four deliverables described in the contract was delivered. Progress was made in other areas as well, particularly in saturated contaminant optimal design, improved economic modeling, and user interface for optimization tools.
3. A computer program has been developed and delivered, together with a short user's guide, which can be used in the design of hydrodynamically contained, three dimensional, groundwater flow systems. MODLP has been released for inclusion in the Argonne Code Library. The software is included in a diskette appended to this report.
4. A prototype user interface for inputting the optimization problem description and automatic generation of the associated data file for MODLP was created. A public domain software package, called Tcl/Tk, that runs on many different computers was used for this computer application. The prototype software is included in a diskette appended to this report.

⇒ We strongly discourage any distribution of this software.
5. A prototype user interface for describing the cost model, relative weighting among cost elements, and selection among different optimizers was

developed. This project was developed for use with Matlab (a commercially licensed software package) and yacc (a well known Unix utility available on many computers). The prototype software is included in a diskette appended to this report.

⇒ **We strongly discourage any distribution of this software.**

6. Progress was made in identifying cost elements that are, and need to be, included in the cost models used in optimal design. Further developments depend upon selection of environmental remediation technologies for unsaturated zone optimal design.
7. Progress was made toward an optimization tool for three dimensional, saturated conditions including solute transport. Key cost elements were identified, a process simulator was selected, and preliminary tests of a possible optimization method was performed.
8. Little progress was made toward an optimization tool for three dimensional, unsaturated zone remediation. Work on this task had just begun when project funds were exhausted.
9. Additional work is required in the construction of user interfaces for the optimization tools being developed under this contract. The prototype user interface built around Matlab and yacc is believed to be a powerful direction.
10. Completing the tasks initiated under this contract will require a total budget of roughly \$450,000. The unsaturated zone project will require a sustained eighteen month effort; interruption of efforts would delay the project by a longer amount of time than the interruption. Because the user interface is dependent upon the unsaturated optimization tools, it is reasonable to estimate a minimum of two years to complete the overall project.

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Appendix A. MODLP Diskette

Appendix B. *xmodopt* Diskette

Appendix C. *optimizer* Diskette

Appendix D. MODLP User Guide

**MODLP Program Description:
A Program for Solving Linear Optimal Hydraulic Control of
Groundwater Contamination Based on MODFLOW Simulation**

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Abstract

MODLP is a computational tool that may help design capture zones for controlling the movement of contaminated groundwater. It creates and solves linear optimization programs that contain constraints on hydraulic head or head differences in a groundwater system. The groundwater domain is represented by the USGS MODFLOW groundwater flow simulation model. This document describes the general structure of the computer program MODLP, the types of constraints that may be imposed, detailed input instructions, interpretation of output, and the interaction with the MODFLOW simulation kernel.

1. INTRODUCTION

MODLP is a computational tool for use in groundwater remediation design. It is a FORTRAN program that incorporates the well known and widely used MODFLOW simulator to represent flow of water in a saturated natural porous medium. MODLP is designed to allow the user to create and solve optimization problems for hydraulic control in groundwater systems. This is accomplished by coupling the groundwater flow simulation MODFLOW with a linear programming (LP) optimization solver. Solving optimization problems involves two steps. First, the simulator is designed and calibrated to match the conditions in the system under study, using available data. The simulator is expected to provide an acceptable representation of the response of the field system to alternate pumping strategies. Second, LP optimization is used to solve for the set of pumping rates and locations that minimizes the weighted sum of pumping while simultaneously satisfying a number of user-specified constraints.

A description of MODFLOW [MacDonald and Harbaugh, 1984] or of its use is far beyond the scope of this document. Tersely, MODFLOW is a three-dimensional, transient or steady-state, saturated groundwater flow simulator developed by the U. S. Geological Survey. It may incorporate a single water table and a variety of commonly encountered, linear boundary and source conditions. The MODFLOW model does not represent solute transport, although it has been extended in a number of proprietary commercial codes to do so.

Users of MODLP are assumed to be familiar (and reasonably comfortable) with simulating groundwater flow using MODFLOW.

MODLP provides a "wrapper" around MODFLOW so that a calibrated groundwater flow model may be interrogated to assess the least cost solution to a groundwater cleanup problem that depends linearly upon the decisions to be taken and for which a set of constraints exist that are linear in the decisions. In its current form, MODLP accommodates vertical or horizontal injection or extraction wells (the wellbore physics are extremely simplified). It is applicable only to confined and leaky aquifer problems (phreatic surface problems are nonlinear and cannot be treated using the LP method).

Specification of the optimization problem requires that the user perform several steps:

- 1) A set of numerical discretization nodes to be considered as candidates for remediation pumping are selected.
- 2) The unit costs for injection and extraction pumping at each candidate well are specified.
- 3) Requirements on the hydraulic behavior of the groundwater system during remediation are selected from a set of possible constraints on head and pumping rates.

2. COUPLING WITH MODFLOW

As previously mentioned, it is assumed that the user of MODLP has already constructed, calibrated, and verified a site-specific model of groundwater flow. To successfully couple this model with MODLP, the MODFLOW must be restricted. The MODFLOW model may contain any of the features of MODFLOW with the following exceptions:

- 1) the model must contain one stress period (i.e., NPER=1).
- 2) the model must run to steady state (i.e., ISS=1).
- 3) the model must be of the constant transmissivity type (i.e., LAYCON=0 for all layers).

The first two exceptions are to maintain computational tractability, while the third is to maintain the linear response of head required by the linear programming formulation.

MODLP contains a complete copy of MODFLOW embedded within it. Only the main program unit, or driver, of MODFLOW has been modified so that it can be invoked repeatedly by the optimization routine. Therefore, a practical application of MODLP follows the construction and calibration of a MODFLOW model. Once an acceptable design-worthy MODFLOW model has been completed, its input files can be used directly by MODLP without modification. A separate input file specific to MODLP must be created for the optimization runs. Note, however, that the MODFLOW input data files are not at all affected by use of MODLP, so they can be preserved for archival and recalibration purposes.

3. CONSTRAINTS AND OBJECTIVE FUNCTIONS IN MODLP

The optimization portion of MODLP always seeks the pumping strategy with the least "cost" associated with it. This cost is defined by the user by placing units costs for injection and extraction pumping at each candidate pumping well. The total cost that is minimized is measured as the sum of the products of the unit costs at each well and the flow rate at the well. Mathematically, the objective function is represented by the weighted sum of withdrawal and recharge rates as

$$\sum_{j \in J} \beta_j q_j \quad (1)$$

where β_j is the relative cost coefficient that related the rate of pumping to the cost of pumping at location j . Note that if injection or extraction are considered at a single spatial location, then there are two decision variables (and two terms in the objective function) corresponding to that one point in space. The use of this cost function presumes that the cost of operation of the hydraulic control system is linearly proportional to the rate of pumping.

Input requirements for each of these constraint types are described below.

MODLP can define two types of constraints on the hydraulic head and one kind of constraint on the pumping rates.

1. An absolute bound may be placed on heads at a point:

$$h_i \geq h_{il}^* \quad (2)$$

or

$$h_i \leq h_{iu}^* \quad (3)$$

where h_{il}^* and h_{iu}^* are specified lower and upper values and h_i is the head at a node where control is to be imposed. Depending on the direction of the inequality, the type of constraint can be used to control excessive drawdown (equation 1a) or mounding (equation 1b) of the piezometric surface.

2. Requirements may be placed on the difference in heads:

$$h_{i1} - h_{i2} \geq d_i^* \quad (4)$$

where d_i^* is the specified bound on head differences, and h_{i1} and h_{i2} are the heads at (often adjoining) node points i_1 and i_2 , respectively. This constraint can be used to

force a gradient in the hydraulic flow field, either horizontally or vertically.

3. Constraints commonly are placed on withdrawal and recharge rates to express bounds on well yield or limitations on the rate at which water can be recharged. Bounds can be imposed on flux rates, either withdrawal or recharge, as follows

$$q_j \leq q_{jmax} \quad (5)$$

where q_j is an individual flux rate at location j and q_{jmax} is the maximum recharge or withdrawal rate respectively that can be achieved at location j .

4. PROGRAM DISTRIBUTION

MODLP is distributed with all FORTRAN source code, together with a sample input set and the corresponding outputs. The source code has been successfully compiled and executed on SUN4, SGI, and IBM RS/6000 workstations and servers, and on DOS/Windows computers.

4.1 Program Structure

The MODLP package consists of a series of modules written in FORTRAN 77, each of which contains a number of subroutines. The module *modlp.f* contains the main program, the input and output subroutines, and the subroutines which construct the linear programming problem.

As part of the formulation of the linear programming coefficient matrix, MODFLOW is called repeatedly. Module *calmod.f* contains the modified main program of MODFLOW (which enables it to be called as a subroutine) and other utility subroutines related to the repeated call of MODFLOW. Modifications to the driver routine of MODFLOW are indicated by lower case text in *calmod.f*, while the original MODFLOW main routine appears in upper case. The remainder of MODFLOW is contained in module *modsub.f*. The subroutines contained in *modsub.f* are unmodified from the copy of MODFLOW distributed by the International Ground Water Modeling Center (Colorado School of Mines, Golden, CO). If an updated version of MODFLOW is incorporated into MODLP, the lower case lines in *calmod.f* indicate most of the changes that will be required to embed the new MODFLOW into MODLP; all other subprograms in the updated MODFLOW replace the current *modsub.f*.

A unique feature of MODLP is the capability for automatic generation of head difference constraints by specification of the outline of a capture zone. The translation of the capture zone definition to constraints is accomplished in module *mkpair.f*.

Once the linear program is formulated, its solution is accomplished using the simplex algorithm [Luenberger, 1984]. Module *lpsub.f* contains an implementation of the simplex algorithm that does not contain many of the efficiency measures and other features present in sophisticated commercial simplex codes. This code is intended for research and educational purposes. Its use for other purposes should be considered with caution.

The program can also generate a standard MPS file which fully describes the LP and can be read by many simplex solution codes. This implementation has been successfully coupled with MINOS 5.1, a product of Stanford University, for example.

4.2 Installing MODLP

To install MODLP on a computer system, choose a directory in which to place the MODLP subdirectory. This directory will be referred to as *\$MODLP_HOME* in this section. Set the current directory to *\$MODLP_HOME* (*cd \$MODLP_HOME*), create a subdirectory *modlp* (*mkdir modlp*),

and move to it (*cd modlp*). Copy all files from the distribution diskette into the directory. Note that the diskette is provided in DOS format; use on another type of computer may require a small change (usually automated on each type of computer) for file format conversion.

Included in the distribution is a file named *Makefile*. This file can be used on Unix systems to compile and link MODLP using the *make* utility. If the FORTRAN compiler is called *f77* and no special libraries are needed, simply type *make*. MODLP will be compiled and linked, and the resulting executable file named *modlp* will be created in the directory *\$MODLP_HOME/modlp*. If the compiler has a different name (e.g., on IBM RS/6000s it is called *xl*) or if some special library is required, then *Makefile* must be edited. At the top of the file are two lines, one starting with the string "*FC =* " and the other starting with "*LLIBS =* ". Append to these lines the compiler or library names (ask a local expert for assistance).

For DOS, Windows, or Windows NT systems *Makefile* may be useful, or it may not be useful. This depends on the compiler that has been installed and whether it uses a *make* or *make-like* utility.

If you intend to use MODLP repeatedly, it will be useful to modify the PATH of the computer to include the *\$MODLP_HOME/modlp* directory.

4.3 Customizing for MODFLOW Application

Manipulation of the various input files required by MODFLOW is performed in subroutine *modio* within module *calmod.f*. Here, the user may introduce OPEN statements for file definition. If the solver within *lpsub.f* is used, then all files used by MODFLOW are rewound in this subroutine at the beginning of the second simulation of flow using the optimized pumping rates.

4.4 Dimensioning

All dimensioning is performed at the top of module MODLP using parameter statements. Internal comments describe the meaning of each parameter. Most of the dimensioning parameters have internal error checking to insure that array dimensions are sufficiently large.

5. INPUT STRUCTURE FOR MODLP-SPECIFIC DATA FILE

The MODFLOW simulator that is embedded in the MODLP package takes input through standard MODFLOW input files as described in the MODFLOW documentation. Code to open MODFLOW input files can be placed in subroutine *modio.f* in module *calmod.f*, although the current implementation assumes that these files will be opened externally. Because MODFLOW is called repeatedly, the MODFLOW files must be rewound to permit re-reading. This is accomplished in subroutine *modio.f* within module *calmod.f* and must be coded by the user.

The optimization input is all contained in a single input file which has the name *opt.in*. The contents of *opt.in* fully describe the optimization formulation. All items in *opt.in* are read in free (i.e., list-directed) format. No adherence to column location is necessary. The units of values in *opt.in* must be consistent with the units used in the user's MODFLOW data set.

The file *opt.in* is organized into five groups of data. No special symbols or delimiters are used within the file to mark the beginning or end of a group.

The first 9 lines of the file *opt.in* comprise GROUP A of the input file. Group A data describe the optimization formulation and directions for its solution. The first line is a title that identifies the problem. The remaining lines contain numerical values describing the optimization problem. These 9 lines are described in the table below.

Note that the coordinates described in line 6 of Group A is only relevant if capture zone lines are defined in Group E. If capture zone lines are not used, then arbitrary values suffice in Group A, line 6. The origin of the coordinate system used in line 6 is assumed to coincide with the external corner of cell (1,1) of the MODFLOW grid. An angle of rotation equal to zero implies that the *x* and *y* coordinates are aligned with the columns and rows, respectively, of the MODFLOW grid.

GROUP A LINE NUMBER	ENTRIES	DESCRIPTION
1	<s1>	String title/description line
2	<n1>	Integer number of candidate wells
3	<n1>	Integer number of head bound constraints
4	<n1>	Integer number of head difference constraints
5	<n1>	Integer number of lines of capture zone information
6	<r1> <r2> <r3>	<r1> = real x coordinate of origin <r2> = real y coordinate of origin <r3> = real angle of rotation of capture zone point coordinates relative to the grid
7	<n1>	Integer flag to calculate/reuse LP coefficient matrix (or response matrix). A value of 1 means compute matrix from scratch using perturbation producing the file <i>jacob</i> . A value of 0 means to use the existing matrix defined in the file <i>jacob</i> . This capability allows the user to repeatedly solve optimization problems with changes to constraint bounds or cost coefficients without recomputing the coefficient matrix. If the number, order, or location of constraints or candidate wells changes, the coefficient matrix must be recomputed from scratch.
8	<n1>	Integer flag to select LP solver. 1 generates MPS deck for use with commercial solver. 2 uses the embedded LP solver <i>lpsub</i> .
9	<n1>	Integer maximum number of LP iterations.

The next set of lines within *opt.in*, GROUP B, describes the candidate wells. The first line in the set is a descriptive, but unused, label. The remaining lines describe each candidate well. The values listed are row number, column number, layer number, flux direction index (1=injection, 2=extraction), upper bound on flux ($q_{i,u}$), and cost coefficient (β_i) used in (1). A lower bound of zero is assumed. If both injection and extraction are to be considered at the same well, then two lines of input are needed, one for each sense. The upper bound on flux may be set to zero to "turn off" the candidate well during successive optimization runs while using the same LP coefficient matrix.

GROUP B LINE NUMBER	ENTRIES	DESCRIPTION
1	<s1>	Descriptive string
2... ...# of candidate wells + 1	<n1> <n2> <n3> <n4> <r1> <r2>	<n1> integer row number <n2> = integer column number <n3> = integer layer number <n4> = flag for sense of pumping 1=injection 2=extraction <r1> = upper bound on flux ($q_{i,u}$) <r2> = cost coefficient (β_i)

The next set of lines, GROUP C, describes the head bound constraints (2) and (3). The first card in the set is a dummy label. Each successive card describes a constraint. The first three values give the row, column, and layer location of the constraint. The absolute value of the last value gives the bounding head value. The sign of the last value has significance. If the sign is negative, the constraint (3) is implied; if the sign is positive then constraint (2) is implied. Thus, this implementation cannot impose bounds on heads below zero.

GROUP C LINE NUMBER	ENTRIES	DESCRIPTION
1	<s1>	String descriptor
2... ...# of head constraints + 1	<n1> <n2> <n3> <r1>	<p><n1> integer row number <n2> = integer column number <n3> = integer layer number <r1> = real head bounding value with sign used as flag.</p> <p>If <r1> is negative, constraint (3) is implied.</p> <p>If <r1> is positive, constraint (2) is implied.</p>

The next set of lines, GROUP D, describes the generalized head difference constraints (4). The first card in the set is a dummy label. Each successive card describes a constraint. The first three values give the row, column, and layer location of cell $i2$ in (4), while the second three values give the row, column, and layer location of cell $i1$ in (4). The final value is d . A value of -999 for d will deactivate the constraint. This may be useful during successive runs using the same LP coefficient matrix.

GROUP D LINE NUMBER	ENTRIES	DESCRIPTION
1	<s1>	String descriptor
2... ...# of head difference constraints + 1	<n1> <n2> <n3> <n4> <n5> <n6> <r1>	<p>For node $i2$ in (4): <n1> integer row number <n2> = integer column number <n3> = integer layer number</p> <p>For node $i1$ in (4): <n4> integer row number <n5> = integer column number <n6> = integer layer number</p> <p><r1> = real head difference d in (4)</p> <p>A value of -999 for d will deactivate the constraint.</p>

GROUP E, the final set of lines, describes the capture zone. MODLP translates the series of lines described here into head difference constraints of the form of (4). Thus, it automatically generates the head difference constraints for all cells along the edge of the capture zone. Input in this section again begins with a dummy card. Each card after this contains three values. If the first value is -9999, then this card describes the beginning of a new capture zone line. The layer in which the line lies is given by the value immediately after the -9999 value. Each capture zone line is described as a series of points. These points are given by the lines that follow the -9999 line and continue until a new -9999 line is reached or all capture zone lines are read. Each line that describes a point has three values. The first two are the x,y coordinates of the point. The last value gives the required gradient along the line formed by the current point and the next point. The gradient value of the last point in the line is ignored. The "inside" of the capture zone is defined to be the left side of the line when one is moving from one point to the next in the list.

GROUP E LINE NUMBER	ENTRIES	DESCRIPTION
1	<s1>	String description
2... ...# of capture zone description lines + 1	<g1> <g2> <g3>	<p>If <g1> = -9999: <g1> = flag indicating start of new capture zone line <g2> = integer layer number in which capture zone lies <g3> = insignificant</p> <p>If <g1> ≠ -9999: <g1> = real x coordinate of point on current capture zone line <g2> = real y coordinate of point on current capture zone line <g3> = real required gradient along the line formed between the current point and the next point</p>

6. OUTPUT INTERPRETATION

MODLP produces up to 4 output streams depending on the LP solver used. Input echo and information describing the generation of the coefficients are written to standard (usually terminal) output.

The output produced by MODFLOW is directed to a file called *modout*. This file will contain the initial MODFLOW solution, a convergence report on each solution used for generating the linear program coefficient matrix, and the final MODFLOW solution.

If the LPSUB solver is selected, then 2 files of output are produced. The main results file is named *solution*. It reports on the solution status and gives the binding constraints and their shadow prices. It also reports the active pumping locations and rates. This output is printed from subroutine OPTOUT within module MODLP and can be modified by the user. The output produced by the formulation solver is written to a file called *solveout*. Its contents give information on the changes to basis that occur at each iteration in the simplex algorithm.

If the MPS solver option is selected, then a file *mpsinput* is created. This file can be directly supplied to a commercial LP solver of the user's choice.

7. DISTRIBUTION TEST PROBLEM

A test problem for MODLP is included with the distribution. A unequally spaced mesh comprising 20 rows, 20, columns, and 2 layers is employed in steady state mode. The strongly implicit procedure (SIP) is used to solve the flow equations. Uniform recharge enters the top layer and head-dependent boundary fluxes occur on two opposing vertical faces of the model region. Wells are allowed at nine locations; five of them may be operated as injection or extraction wells, whereas the remaining four wells can be used for extraction only. The cost of operating each well per unit discharge rate is identical. The optimization problem is to minimize the total pumping rate from the nine wells, each of which has limits on pumping rate, such that a capture zone is created. In addition, there are three constraints to insure that heads remain below 35 feet at three spatial locations and three locations at which head differences (discrete versions of gradient constraints) are imposed. The input data are contained in file *sam.in*.

The origin of the coordinate system is in the lower left corner of the grid, in accordance with usual Cartesian coordinates. The indices of rows and columns of the grid also begin in that corner. The locations of constraints and candidate wells are given in the file *sam.in*. Note that the third line of input in the capture zone line group indicates a gradient requirement of -10000. This value is easily satisfied for the sample problem configuration. It effectively turns off the constraints along the line between points (3950, 2950) and (4750,2950).

Execution of the sample problem requires files defined with default name *fort.n* where n has values 1, 8, 11, 14, 15, 19, and 23. Execution produces output to the screen and to files *modout*, *solveout*, and *solution*. In addition, the program produces *jacob*, an unformatted file containing the linear programming coefficient matrix. This file is used for input to subsequent runs if the coefficient equations do not change. The program also produces *solution.all*, which shows more details of the LP solution. To insure proper execution of the program, the user should run MODLP with test problem described by *sam_opt.in*. The distribution files *solution.sam*, *solveout.sam*, and *modout.sam* should be identical (barring roundoff error due to compiler and hardware differences) to the corresponding files produced by such a test run.

The output from the sample problem indicates that only two of the constraints are binding at the optimal solution. All other constraints are satisfied as inequalities. The sample output also shows that only two of the 14 candidate wells have been selected and that both of them are operated as extraction wells.

8. REFERENCES

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