Figure 5-18: Shallow Particles, Contain Shallow 20-ppb Plume, \& 500 gpm for Deep 20-ppb plume ( 1573 gpm, 3 new wells, 1 existing well)


A "+" symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Shallow particles originate half-way down in layer 1.

Figure 5-19: Deep Particles, Contain Shallow 20-ppb Plume, \& 500 gpm for Deep 20-ppb plume ( $1573 \mathrm{gpm}, 3$ new wells, 1 existing well)


Figure 5-20: Shallow Particles, Contain Shallow 20-ppb \& 50-ppb Plumes, \& 500 gpm for Deep 20-ppb plume ( $2620 \mathrm{gpm}, 6$ new wells, 0 existing wells)


Figure 5-21: Deep Particles, Contain Shallow 20-ppb \& 50-ppb Plumes, \& 500 gpm for Deep 20-ppb plume ( 2620 gpm, 6 new wells, 0 existing wells)


A " + " symbol indicates that a particle starting at that location is captured by one of the remediation wells, based on particle tracking with MODPATH. Deep particles originate half-way down in layer 2.




- POTENTIAL ADDITIONAL WELL

HEAD DIFFERENCE CONSTRAINT

RELATIVE GRADIENT CONSTRAINT
SHALLOW CORE ZONE TARGET VOCs > $1000 \mathrm{ug} / \mathrm{L}$

SHALLOW-INTERMEDIATE CORE ZONE: TARGET VOCs > 1000 ug/L

INTERMEDIATE CORE ZONE: TARGET VOCs > 1000 ug/L
DEEP CORE ZONE:
TARGET VOCs > 1000 ug/L

------- PROPERTY BOUNDARY


Figure 6-5. Solutions for multiple toe wells, Offutt.



## TABLES

Table 4-1. Current system, Kentucky.

## Site: Kentucky Scenario: Current System

Discount Rate: 0.05

|  | Up-Front Costs | Annual Costs | \# Years | Talo Annual Costs | Total Costs |
| :---: | :---: | :---: | :---: | :---: | :---: |
| O\&M Costs |  |  |  |  |  |
| -Electric | \$0 | \$200,000 | 20 | \$2,617,064 | \$2,617,064 |
| -Materials (pH adjustment) | \$0 | \$100,000 | 20 | \$1,308,532 | \$1,308,532 |
| -Maintenance | \$0 | \$50,000 | 20 | \$654,266 | \$654,266 |
| -Discharge Fees | \$0 | \$0 | 20 | \$0 | \$0 |
| -Annual O\&M | \$0 | \$250,000 | 20 | \$3,271,330 | \$3,271,330 |
| -Analytical | \$0 | \$0 | 20 | \$0 | \$0 |
| -Steam | \$0 | \$1,200,000 | 20 | \$15,702,385 | \$15,702,385 |
| -Other 2 | \$0 | \$0 | 20 | \$0 | \$0 |
| -Other 3 | \$0 | \$0 | 20 | \$0 | \$0 |
|  |  |  |  |  |  |
| Costs of Analysis |  |  |  |  |  |
| -Flow Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Transport Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Optimization | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
| System Modification Costs |  |  |  |  |  |
|  |  |  |  |  |  |
| -Engineering Design | \$0 | \$0 |  | \$0 | \$0 |
| -Regulatory Process | \$0 | \$0 |  | \$0 | \$0 |
| -New wells/pipes/equipment | \$0 | \$0 |  | \$0 | \$0 |
| -Increased Monitoring | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 2 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 3 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
| Total Costs | \$0 | \$1,800,000 |  | \$23,553,578 | \$23,553,578 |

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

## Assumptions

Analytical costs not included.

Table 4-2. Summary of design well rates and maximum observed well rates (6/97 to 11/97), Kentucky.

| Well | Design Rate (gpm) | Max Rate (gpm) | Comments |
| :---: | :---: | :---: | :---: |
| bw-1928 | 7.84 | 18.16 |  |
| bw-1929 | 36.67 | 15.62 |  |
| bw-1930 | 12.16 | 25.11 |  |
| bw-1931 | 2.73 | 15.56 |  |
| bw-1932 | 7.69 | 18.10 |  |
| bw-1933 | 48.57 | 36.55 |  |
| bw-1934 | 43.58 | 43.11 |  |
| bw-1935 | 42.59 | 32.42 |  |
| bw-1936 | 58.54 | 62.87 |  |
| bw-1937 | 62.90 | 61.84 |  |
| bw-1938 | 54.44 | 36.19 |  |
| bw-1939 | 29.71 | 34.63 |  |
| bw-1940 | 35.74 | 35.42 |  |
| bw-1941 | 37.97 | 33.36 |  |
| bw-1944 | 19.74 | 34.80 |  |
| bw-1945 | 19.79 | 35.21 |  |
| bw-1946 | 20.05 | 35.56 |  |
| bw-1947 | 8.78 | 35.99 |  |
| bw-1948 | N/A | 11.64 | Installed after original design |
| bw-1949 | N/A | 29.78 | Installed after original design |
| bw-1950 | N/A | 36.56 | Installed after original design |
| bw-1952 | N/A | 2.04 | Installed after original design |
| bw-1953 | N/A | 10.09 | Installed after original design |
| BW Subtotal | 549.49 | 700.61 |  |
| sw-1918 | 21.14 | 7.97 |  |
| sw-1920 | 8.26 | 20.80 |  |
| sw-1921 | 7.90 | 13.03 |  |
| sw-1924 | 81.29 | 63.84 |  |
| sw-1925 | 13.77 | 6.29 |  |
| sw-1926 | 4.00 | 10.61 |  |
| sw-1942 | 21.19 | 36.64 |  |
| sw-1943 | 13.04 | 30.91 |  |
| SW Subtotal | 170.59 | 190.01 |  |
| ow-1914 | 12.00 | 6.96 |  |
| ow-1915 | 11.90 | 6.84 |  |
| ow-1916 | 12.41 | 7.22 |  |
| ow-1917 | 14.91 | 11.13 |  |
| ow-1919 | 21.82 | 20.11 |  |
| ow-1922 | 14.70 | 43.83 |  |
| ow-1923 | 31.69 | 39.96 |  |
| OW Subtotal | 131.67 | 143.17 |  |

Note: Max Rate refers to maximum observed rate between 6/97 and 11/97, based on daily measurements.

Table 5-1. Current system, Tooele.

## Screening Analysis

Site: Tooele

## Scenario: Current System

Discount Rate: 0.05

|  | Up-Front Costs | Annual Costs | \# Years | Total of Annual Costs | Total Costs |
| :---: | :---: | :---: | :---: | :---: | :---: |
| O\&M Costs |  |  |  |  |  |
| -Electric | \$0 | \$1,000,000 | 20 | \$13,085,321 | \$13,085,321 |
| -Materials (Sodium Metaphosphate) | \$0 | \$200,000 | 20 | \$2,617,064 | \$2,617,064 |
| -Maintenance | \$0 | \$30,000 | 20 | \$392,560 | \$392,560 |
| -Discharge Fees | \$0 | \$0 | 20 | \$0 | \$0 |
| -Annual O\&M | \$0 | \$500,000 | 20 | \$6,542,660 | \$6,542,660 |
| -Analytical | \$0 | \$80,000 | 20 | \$1,046,826 | \$1,046,826 |
| -Other 1 | \$0 | \$0 | 20 | \$0 | \$0 |
| -Other 2 | \$0 | \$0 | 20 | \$0 | \$0 |
| -Other 3 | \$0 | \$0 | 20 | \$0 | \$0 |
|  |  |  |  |  |  |
| Costs of Analysis |  |  |  |  |  |
| -Flow Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Transport Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Optimization | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| System Modification Costs |  |  |  |  |  |
| -Engineering Design | \$0 | \$0 |  | \$0 | \$0 |
| -Regulatory Process | \$0 | \$0 |  | \$0 | \$0 |
| -New wells/pipes/equipment | \$0 | \$0 |  | \$0 | \$0 |
| -Increased Monitoring | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 2 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 3 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
| Total Costs | \$0 | \$1,810,000 |  | \$23,684,431 | \$23,684,431 |

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Assumptions
None

Table 5-2. Example calculation for "Total Managed Cost", Tooele.

Calculate Total Managed Cost (Example)
Site: Tooele
Scenario: 12 new wells, total of $\mathbf{4 2 0 0}$ gpm
\# New Wells 12
Pumping Rate (gpm) 4200
Discount Rate: 0.05

|  | Up-Front Costs | Annual Costs | \# YearsTotal of Annual <br> Costs |  | Total Costs |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| New Wells (\$300K/well) | \$3,600,000 | \$0 | 0 | \$0 | \$3,600,000 |
| Managed Annual Costs (\$150/yr/gpm) | \$0 | \$630,000 | 20 | \$8,243,752 | \$8,243,752 |
|  |  |  |  |  |  |
| Total Costs | \$3,600,000 | \$630,000 |  | \$8,243,752 | \$11,843,752 |

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Table 6-1. Current system, Offutt: one new core well, 100 gpm at LF wells.

Screening Analysis

## Site: Offutt Scenario: Current System (Add 1 new core zone well, pump 200 gpm from 4 wells)

Discount Rate: 0.05

|  | Up-Front Costs | Annual Costs | \# Years | Total of Annual Costs | Total Costs |
| :---: | :---: | :---: | :---: | :---: | :---: |
| O\&M Costs |  |  |  |  |  |
| -Electric | \$0 | \$2,000 | 20 | \$26,171 | \$26,171 |
| -Materials | \$0 | \$0 | 20 | \$0 | \$0 |
| -Maintenance (Labor) | \$0 | \$12,000 | 20 | \$157,024 | \$157,024 |
| -Discharge (Core \& LF $150 \mathrm{gpm}, 20 \mathrm{yrs}$ ) | \$0 | \$60,000 | 20 | \$785,119 | \$785,119 |
| -Annual O\&M | \$0 | \$3,000 | 20 | \$39,256 | \$39,256 |
| -Analytical | \$0 | \$25,000 | 20 | \$327,133 | \$327,133 |
| -Discharge (Toe Well, $50 \mathrm{gpm}, 10 \mathrm{yrs}$ ) | \$0 | \$20,000 | 10 | \$162,156 | \$162,156 |
| -Other 2 | \$0 | \$0 | 20 | \$0 | \$0 |
| -Other 3 | \$0 | \$0 | 20 | \$0 | \$0 |
|  |  |  |  |  |  |
| Costs of Analysis |  |  |  |  |  |
| -Flow Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Transport Modeling | \$0 | \$0 |  | \$0 | \$0 |
| -Optimization | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
| System Modification Costs |  |  |  |  |  |
|  |  |  |  |  |  |
| -Fixed Construction/All Scenarios | \$47,000 | \$0 |  | \$0 | \$47,000 |
| -Regulatory Process | \$0 | \$0 |  | \$0 | \$0 |
| -New wells/pipes/equipment | \$40,000 | \$0 |  | \$0 | \$40,000 |
| -Increased Monitoring | \$0 | \$0 |  | \$0 | \$0 |
| -Other 1 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 2 | \$0 | \$0 |  | \$0 | \$0 |
| -Other 3 | \$0 | \$0 |  | \$0 | \$0 |
|  |  |  |  |  |  |
| Total Costs | \$87,000 | \$122,000 |  | \$1,496,859 | \$1,583,859 |

Note: All costs are in present-day dollars. The discount rate is applied to annual costs to calculate the Net Present Value (NPV). The PV function in Microsoft Excel was utilized to calculate NPV, with payments applied at the beginning of each year.

Assumptions
Toe well can be shut off in 10 yrs

## APPENDIX A:

## Overview of MODMAN

## MODMAN Code History

MODMAN (Greenwald, 1998a) is a FORTRAN code developed by HSI GeoTrans that adds optimization capability to the U.S.G.S. finite-difference model for groundwater flow simulation in three dimensions, called MODFLOW-96 (Harbaugh and McDonald, 1996a,b). MODMAN, in conjunction with optimization software, yields answers to the following groundwater management questions: (1) where should pumping and injection wells be located, and (2) at what rate should water be extracted or injected at each well? The optimal solution maximizes or minimizes a userdefined objective function and satisfies all user-defined constraints. A typical objective may be to maximize the total pumping rate from all wells, while constraints might include upper and lower limits on heads, gradients, and pumping rates. A variety of objectives and constraints are available to the user, allowing many types of groundwater management issues to be considered.

MODMAN Version 1.5 was originally developed for the South Florida Water Management District (SFWMD) in 1989-1990. Emphasis was placed on the solution of water supply problems. The majority of code conceptualization, code de-bugging, and code documentation to date has been performed under contract to SFWMD. MODMAN Version 2.0, developed for the USEPA in 1990, included additional features for the solution of groundwater management problems related to plume containment and plume removal. MODMAN Version 2.1 was developed in 1992 for SFWMD to allow wells to be constrained to pump or inject only at their upper or lower allowable rates, if they are selected to pump at all in the optimal solution. MODMAN Version 3.0 was linked to a version of MODFLOW distributed by the International Ground Water Modeling Center (IGWMC). The current version, MODMAN Version 4.0, has been developed for the USEPA and is linked directly with the MODFLOW-96 code A preprocessor for reading and writing MOMAN input files, and running MODMAN and LINDO from a user shell, is also now available (Greenwald, 1998b). This preprocessor runs in the Microsoft Windows environment.

The MODMAN code logic is an extension of AQMAN (Lefkoff and Gorelick, 1987), a code developed by the U.S. Geological Survey for two-dimensional groundwater management modeling. However, MODMAN is a significantly more comprehensive package than AQMAN, offering a large variety of management options and input/output features not available with the AQMAN code.

## Flowchart for Executing MODMAN

A flowchart describing the optimization process is presented in Figure A-1. First, a groundwater model is calibrated with MODFLOW. A management problem is formulated and a MODMAN input file indicating user-defined choices for the objective function and constraints is created by the user. The decision variables are the pumping and/or injection rates at potential well locations. MODMAN utilizes the response matrix technique to transform the groundwater management problem into a linear or mixed-integer program. To perform the response matrix technique, a slightly modified version of MODFLOW is called repeatedly as a subroutine. The linear or mixedinteger program is written to an ASCII file in MPS (Mathematical Programming System) format. At this point, the execution of MODMAN in "mode 1 " is complete.

The next step is to solve the linear or mixed-integer program. The MPS file is read into the optimization code LINDO (Lindo Systems, 1996) to determine the optimal solution. Specific LINDO commands generate an output file containing the optimal solution. MODMAN is then executed a second time ("mode 2") to read this file and postprocess the optimal results. As part of the post-processing, MODMAN automatically inserts the optimal well rates into MODFLOW, performs a simulation based on the optimal well rates, indicates which constraints are "binding" (exactly satisfied by the optimal solution), and indicates if nonlinearities have significantly affected the optimization
process. A methodology is suggested in the User's Guide (Greenwald, 1998a) to solve problems where nonlinearities significantly affect optimal results.


Figure A-1. General flowchart for executing MODMAN.

## Linear Response Theory in Groundwater Systems Upon Which MODMAN is Based

Linear response theory in groundwater systems is based on the principle of linear superposition. The principle of linear superposition is two-fold in nature:

- multiplication of a well rate by a factor increases drawdown induced by that well by the same factor; and
- drawdown induced by more than one well is equal to the sum of drawdowns induced by each individual well.

Linear superposition, when applicable, is valid for both steady-state and transient groundwater systems. Linear superposition is not strictly applicable in unconfined systems, but often may be reasonably applied. Likewise, in some systems where river leakage, drains, or evapotranspiration are significant components, linear superposition is not strictly applicable but may often be reasonably applied. A detailed explanation of linear versus nonlinear responses in groundwater systems is presented in the User's Guide (Greenwald, 1998a).

## Concept Of The Response Matrix

A response matrix, generated on the basis of linear superposition, allows drawdown induced by one or more wells to be calculated with matrix multiplication. For example, drawdown at three control locations, induced by two wells in a steady-state system, is calculated as follows:

where
$\mathrm{s}_{\mathrm{i}}=$ drawdown at control location $\mathrm{i}(1,2$, or 3 )
$\mathrm{Q}_{\mathrm{j}}=$ rate at well j (A or B)
$\mathrm{R}_{\mathrm{ij}}=$ drawdown response at location i to a unit stress at well j
Once the response matrix is known, any set of well rates may be entered and the resulting drawdowns calculated.
With a response matrix, drawdowns induced by wells are defined as linear combinations of well rates. This allows implementation of linear programming methodology, with well rates as the decision variables. The objective function and each constraint are written in terms of well rates, either directly or in terms of drawdowns (which are linearly determined from well rates). Constraints pertaining to heads, head differences, gradients and velocities may all be defined in terms of drawdown, and therefore be included in the optimization process.

The first step for generating the response matrix is to define control locations. These are locations where one or more hydrogeologic constraints, such as limits on head, will be applied. The second step is to define the location of each managed well (i.e., each decision well). Wells where rates are fixed, and therefore not part of the decisionmaking process, are not managed wells and are called fixed wells. The third step is to compute the unmanaged head (explained below), in each stress period, at each control location. Then, one groundwater flow simulation is performed for each managed well location, to determine the coefficients for the response matrix.

## Unmanaged Heads

Unmanaged heads refer to simulated heads resulting from unmanaged (i.e., background) flow conditions. Unmanaged flow conditions are created when all managed wells are turned off for the entire simulation. Unmanaged heads are a function of fixed well rates, boundary conditions, initial conditions (in transient cases), and hydrogeologic properties.

Unmanaged heads must be calculated before the response matrix can be generated. The reason is that drawdowns induced by each managed well must be discernible from drawdowns due to other factors, such as fixed wells. For instance, to determine drawdown induced by a well, it is first necessary to simulate heads with no pumping at the well (unmanaged head). Drawdown induced by rate Q at the well is the difference between heads resulting from rate Q and the unmanaged heads. All boundary effects, fixed wells, and hydrogeologic conditions are accounted for in both simulations. Then the drawdown induced by any rate at that particular well can be calculated, using the principle of linear superposition.

## Concept Of A Unit Stress And Scaling

The coefficients in the response matrix are calculated for each managed well by applying a stress at that well, and determining the drawdown at each control location induced by that stress. The stress applied at a managed well to generate these coefficients is called the unit stress, or unit rate. The drawdown at each control location induced by the unit stress is called the drawdown response:

$$
\begin{array}{cccc}
\text { drawdown } \\
\text { response }
\end{array} \quad=\quad \text { unmanaged } \quad-\quad \text { head resulting from }
$$

The unit response is defined as:

$$
\text { unit response }=\text { drawdown response } / \text { unit rate }
$$

and is interpreted as drawdown induced by a rate of one unit. Drawdown due to any other well rate is then calculated as:

$$
\text { induced drawdown } \quad=\text { unit response } * \text { well rate. }
$$

The magnitude of the unit stress can be quite significant with regard to scaling. In general, a unit rate should be chosen that is the same magnitude as expected well rates. For example, if actual well rates are constrained to be between -1000 and -6000 units, a unit rate of -1000 units is much better than a unit rate of -1 unit. One reason is that a unit rate of -1 unit may yield such small drawdown responses that FORTRAN precision errors and MODFLOW convergence criteria become significant. Another reason is that a small unit rate will produce very small coefficients in the response matrix, which is not good for the LP/MIP solver (coefficients close to one are preferred for matrix inversions used to solve the LP or MIP). Both of these situations would be termed "scaling problems".

## Repeated Simulations (Steady-State and Transient Cases)

To determine response coefficients for a managed well in a steady-state case, a unit rate is applied at that well while
all other managed wells are turned off (rate of zero). This procedure is repeated for each managed well, with one simulation for each managed well.

For transient cases the same procedure is followed, but the unit rate is only applied in stress period 1. All stress periods are required to be of equal length. Drawdown responses in all periods are calculated in terms of a unit rate applied in stress period 1. The reason is that drawdown in each period is not only induced by pumping in that period, but also by pumping in previous periods. For instance, drawdown in period 2 is due to pumping in period 2 and pumping in period 1. Because stress periods are of equal length, drawdown in period 3 due to a stress in period 2 is the same as drawdown in period 2 due to the same stress in period 1. This feature allows the entire response matrix for transient systems to be constructed with one simulation per managed well, by applying unit stresses in period 1 only.

This concept is best illustrated with an example. Suppose there are two wells (A and B), two control locations (x and y), and three stress periods. First, unmanaged heads are calculated with MODFLOW, setting rates at wells A and B to zero for all three stress periods. Then drawdown responses for well A are calculated with MODFLOW, for the entire three periods, with a unit rate applied at well A during period 1 only, and no pumping at well B . The process is repeated for well B , with well A not pumping. Suppose the drawdown responses, at the end of each stress period, are as follows:


Note that drawdown responses are negative. The sign convention for drawdown is positive for head lowered below a datum and negative for head raised above a datum. The sign convention for pumpage is negative for withdrawal and positive for injection. A negative pumpage (withdrawal) will create a positive drawdown and vice versa.
Accordingly, the drawdown responses (matrix generated from a unit stress) will always be negative. The response matrix for this example, in matrix notation, is:


Managed drawdown, $s$, at each of the control points ( $x$ or $y$ ) can be calculated from the response matrix for any time period. For instance, managed drawdown at point x after period 2 is:

$$
\begin{array}{ccc}
\mathrm{s}_{\mathrm{x}, 2}= & -0.20 \mathrm{Q}_{\mathrm{A}, 1}+-0.40 \mathrm{Q}_{\mathrm{B}, 1} & + \\
& --0.50 \mathrm{Q}_{\mathrm{A}, 2}+-0.75 \mathrm{Q}_{\mathrm{B}, 2} \\
& \text {--due to pumping in--- } & \text {--due to pumping in--- } \\
\text { stress period 1 } & \text { stress period } 2
\end{array}
$$

Note the predominance of zeroes above the main diagonal of the response matrix. This results because drawdown is due to current and previous pumpage, but not future pumpage. In the above example, drawdowns in time period 1 only depend on pumping in period 1 , while drawdowns in period 2 are based on pumping in periods 1 and 2 . Note the repetition of blocks within the response matrix. This structure is made possible by the fact that stress periods are of equal length, and allows efficient storage of the response matrix in the MODMAN code. Also note that the response matrix is fully generated by applying a unit stress, at each decision well, in the first stress period only.

## ApPENDIX B:

## Overview of Simulation-Management Methods Incorporating Transport Simulations

Hydraulic optimization is based on simulation of groundwater flow. In many cases, the management objectives or constraints at a site may involve terms that cannot be rigorously evaluated with a groundwater flow model, such as contaminant concentrations and/or cleanup time. In those cases, solute transport models can be developed to predict contaminant concentrations over space and/or time, and simulation-management techniques based on the results of the contaminant transport simulations can be applied.

Many hydraulic optimization techniques (e.g., those employed by MODMAN) utilize the principle of linear superposition to transform the groundwater management problem into a linear program (see Appendix A). This is possible because, when linear superposition applies, drawdown is directly proportional to pumping rate. Unfortunately, there is no such linear relationship between concentrations and pumping rates. Increasing pumping rate by a factor of two does not decrease concentrations by a factor of two. Therefore, simulation-management problems involving contaminant transport require optimization techniques that are significantly more complex than linear programming.

Since the mid-1980's, a large number of transport-based simulation-management approaches have been described in the literature. These techniques are typically computer-intensive, but with improved algorithms and constantly improving computer speeds, these techniques are likely to become more mainstream within the next several years. A full review of transport-based simulation-management modeling is well beyond the scope of this report. The interested reader can begin with some of the references indicated in Appendix I of this report. A partial listing of researchers that are particularly active in code development for transport-based simulation-management modeling is as follows:

David Dougherty<br>Richard Peralta<br>Christine Shoemaker<br>Brian Wagner<br>Chunmiao Zheng

Contact information for these individuals is presented in Appendix I.

## Appendix C:

## Overview of Simulation-Management Methods Incorporating Uncertainty and/or Risk

The applications of hydraulic optimization presented in this study are based on deterministic groundwater flow simulations (i.e., model parameters are assumed to be known precisely). Impacts to mathematical optimal solutions from uncertainties associated with the groundwater flow model are not accounted for. Stochastic groundwater management tools are required to account for:
(1) parameter uncertainty; and/or
(2) spatially variable aquifer properties that can only be represented statistically.

Coupling of stochastic techniques with simulation-management models can allow uncertainty and risk to be incorporated into the optimization algorithm. For example, one can specify that constraints be satisfied within a specified reliability (e.g., constraints satisfied with $95 \%$ reliability). Another example is to specify constraints that satisfy multiple potential realizations for spatial distribution of key aquifer parameters (e.g., hydraulic conductivity), rather than one realization in a deterministic model. Stochastic approaches to simulation-management modeling have been applied to both hydraulic optimization and transport optimization problems.

A full review of this topic is well beyond the scope of this report. A brief description is provided in Appendix B of Gorelick et. al. (1993). An excellent resource for this area of research is Brian Wagner at the U.S.G.S. (see Appendix I for contact information).

## APPENDIX D:

## Partial Listing of MODMAN Applications

Douthitt, Jeff W. And Bruce E. Phillips, 1994, "Model Assisted Design of a Groundwater Pump and Treat System at the Paducah Gaseous Diffusion Plant", Toxic Substances and the Hydrologic Sciences, American Institute of Hydrology, pp. 346 to 365.

Greenwald, Robert M. and Joost C. Herweijer, Ira Star, Mark Gallagher, and Allan L. Dreher, 1992, "Optimization of Well Locations and Rates for Containment of Contaminants Utilizing an Automated Management Routine Coupled to MODFLOW: A Case History", Solving Ground Water Problems With Models, Dallas, Texas, February 1992.

Hagemeyer, Todd R., Peter F. Andersen, Robert M. Greenwald, and Jay L. Clausen, 1993, "Evaluation of Alternative Plume Containment Designs at the Paducah Gaseous Diffusion Plant Using MODMAN, A Well Pumpage Optimization Module for MODFLOW', IGWMC Modeling Conference, Golden, Colorado, June 1993.

Johnson, Kevin D. and James D. Bowen, 1993, "Trade-Offs Between Pumping and Slurry Walls Under Changing Hydraulic Parameters", IGWMC Modeling Conference, Golden, Colorado, June 1993

McCready, Roger W. And Robert M. Greenwald, 1997, "Pump-and-Treat Well Location and Rate Optimization Using MODFLOW and MODMAN: A Case Study", Midwest Groundwater Conference, Coralville, Iowa, October 1997 (Abstract Only).

Russell, K.T. and A.J. Rabideau, "Decision Analysis for Pump-and-Treat Design", Ground Water Monitoring and Remediation (in press).

Russell, K.T. and A.J. Rabideau, "Simulating the Reliability of Pump-and-treat Systems", Ground Water Monitoring and Remediation (in review).

## Appendix E:

## SAMPLE MODMAN InPut: KENTUCKY





```
    0
SET8: Balance Constraints
    0
SET9: Integer Constraints
1 B
1
L
18
1 8
/limit # BW wells to 18 or less
1
SET10: Objective Function
1 r 43
1
1 2 -5.194E-03
1 4 -5.194E-03
1 5 -5.194E-03
1 6 -5.194E-03
1 7 -5.194E-03
1 8 -5.194E-03
1 9 -5.194E-03
10-5.194E-03
11-5.194E-03
12 -5.194E-03
13 -5.194E-03
14 -5.194E-03
1 15 -5.194E-03
1 16 -5.194E-03
17 -5.194E-03
1 18 -5.194E-03
19-5.194E-03
20 -5.194E-03
21 -5.194E-03
22-5.194E-03
23-5.194E-03
24-5.194E-03
25 -5.194E-03
26 -5.194E-03
1 27 -5.194E-03
28-5.194E-03
29-5.194E-03
-30-5.194E-03
31 -5.194E-03
32 -5.194E-03
1 33-5.194E-03
34-5.194E-03
35 -5.194E-03
36-5.194E-03
37-5.194E-03
38-5.194E-03
39-5.194E-03
40 -5.194E-03
41 -5.194E-03
42 -5.194E-03
1 43-5.194E-03
```


## Appendix F:

## SAMPLE MODMAN InPUT: Tooele






|  | 113 | 2 | 91 | 54 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 114 | 2 | 91 | 53 |  |  |  |
| SET4: Head Limits |  |  |  |  |  |  |  |
| SET5: Head Difference Limits |  |  |  |  |  |  |  |
| 2 | 1 | 1 | 28 | 29 | . 02 | 1. $\mathrm{E}+20$ | /*first 3 are shallow |
|  | 2 | 1 | 60 | 61 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 3 | 1 | 62 | 63 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 4 | 1 | 85 | 86 | . 02 | 1. $\mathrm{E}+20$ | /*next 9 are deep |
|  | 5 | 1 | 87 | 88 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 6 | 1 | 89 | 90 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 7 | 1 | 91 | 92 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 8 | 1 | 105 | 106 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 9 | 1 | 107 | 108 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 10 | 1 | 109 | 110 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 11 | 1 | 111 | 112 | . 02 | 1. $\mathrm{E}+20$ |  |
|  | 12 | 1 | 113 | 114 | . 02 | 1. $\mathrm{E}+20$ |  |
| SET6: Drawdown Limits |  |  |  |  |  |  |  |
| SET7A: Gradient Limits |  |  |  |  |  |  |  |
|  | 1 | 1 | 1 | 2 | -10.00 | 1. $\mathrm{E}+20$ | /*first 38 are shallow |
|  | 2 | 1 | 1 | 3 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 3 | 1 | 4 | 5 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 4 | 1 | 4 | 6 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 5 | 1 | 7 | 8 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 6 | 1 | 7 | 9 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 7 | 1 | 10 | 11 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 8 | 1 | 10 | 12 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 9 | 1 | 13 | 14 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 10 | 1 | 13 | 15 | 1. E-04 | 1. $\mathrm{E}+20$ |  |
|  | 11 | 1 | 16 | 17 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 12 | 1 | 16 | 18 | 1. E-04 | 1. $\mathrm{E}+20$ |  |
|  | 13 | 1 | 19 | 20 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 14 | 1 | 19 | 21 | 1. E-04 | 1. $\mathrm{E}+20$ |  |
|  | 15 | 1 | 22 | 23 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 16 | 1 | 22 | 24 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 17 | 1 | 25 | 26 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 18 | 1 | 25 | 27 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 19 | 1 | 30 | 31 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 20 | 1 | 30 | 32 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 21 | 1 | 33 | 34 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 22 | 1 | 33 | 35 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 23 | 1 | 36 | 37 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 24 | 1 | 36 | 38 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 25 | 1 | 39 | 40 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 26 | 1 | 39 | 41 | 1. E-04 | 1. $\mathrm{E}+20$ |  |
|  | 27 | 1 | 42 | 43 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 28 | 1 | 42 | 44 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 29 | 1 | 45 | 46 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 30 | 1 | 45 | 47 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 31 | 1 | 48 | 49 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 32 | 1 | 48 | 50 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 33 | 1 | 51 | 52 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 34 | 1 | 51 | 53 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 35 | 1 | 54 | 55 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 36 | 1 | 54 | 56 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 37 | 1 | 57 | 58 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 38 | 1 | 57 | 59 | 1.E-04 | 1. $\mathrm{E}+20$ | /* next 22 are deep |
|  | 39 | 1 | 64 | 65 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 40 | 1 | 64 | 66 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 41 | 1 | 67 | 68 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 42 | 1 | 67 | 69 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 43 | 1 | 70 | 71 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 44 | 1 | 70 | 72 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 45 | 1 | 73 | 74 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 46 | 1 | 73 | 75 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 47 | 1 | 76 | 77 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 48 | 1 | 76 | 78 | 1.E-04 | 1. $\mathrm{E}+20$ |  |
|  | 49 | 1 | 79 | 80 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 50 | 1 | 79 | 81 | 1.E-04 | 1. $\mathrm{E}+20$ |  |



| 1 | 30 | 1.00 |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 31 | -1.22 |  |  |  |  |
|  | 11 | C | E | $0 . \mathrm{E}+00$ | 2 |  |
| 1 | 32 | 1.00 |  |  |  |  |
| 1 | 33 | -1.22 |  |  |  |  |
|  | 12 | C | E | $0 . \mathrm{E}+00$ | 2 |  |
| 1 | 35 | 1.00 |  |  |  |  |
| 1 | 36 | -1.50 |  |  |  |  |
|  | 13 | C | E | $0 . \mathrm{E}+00$ | 2 |  |
| 1 | 37 | 1.00 |  |  |  |  |
| 1 | 38 | -3.00 |  |  |  |  |
|  | 14 | C | E | $0 . \mathrm{E}+00$ | 2 |  |
| 1 | 41 | 1.00 |  |  |  |  |
| 1 | 42 | -4.00 |  |  |  |  |
|  | 15 | C | L | 0.E+00 | 23 | /*sums existing extraction wells |
| 1 | 1 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 2 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 3 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 4 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 5 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 6 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 7 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 8 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 9 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 10 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 11 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 12 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 13 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 14 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 15 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 16 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 17 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 18 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 19 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 20 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 21 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 22 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 23 | $5.194 \mathrm{E}-03$ |  |  |  |  |
|  | 16 | C | L | 0.E+00 | 20 | /*sums new shallow extraction |
| 1 | 43 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 44 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 45 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 46 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 47 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 48 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 49 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 50 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 51 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 52 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 53 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 54 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 55 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 56 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 57 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 58 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 59 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 60 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 61 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 62 | $5.194 \mathrm{E}-03$ |  |  |  |  |
|  | 17 | C | L | $0 . \mathrm{E}+00$ | 18 | /*sums new deep extraction |
| 1 | 63 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 64 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 65 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 66 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 67 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 68 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 69 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 70 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 71 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 72 | $5.194 \mathrm{E}-03$ |  |  |  |  |
| 1 | 73 | $5.194 \mathrm{E}-03$ |  |  |  |  |




| 1 | 71 | $-5.194 \mathrm{E}-03$ |  | /*factor converts to gpm, neg allows minimize |
| :--- | :--- | :--- | :--- | :--- |
| 1 | 72 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 73 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 74 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 75 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 76 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 77 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 78 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 79 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |
| 1 | 80 | $-5.194 \mathrm{E}-03$ | /*factor converts to gpm, neg allows minimize |  |

$171-5.194 \mathrm{E}-03$
$172-5.194 \mathrm{E}-03$
$173-5.194 \mathrm{E}-03$
$174-5.194 \mathrm{E}-03$
$175-5.194 \mathrm{E}-03$
$176-5.194 \mathrm{E}-03$
$177-5.194 \mathrm{E}-03$
$178-5.194 \mathrm{E}-03$
$180-5.194 \mathrm{E}-03$
/*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize *factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize /*factor converts to gpm, neg allows minimize

## ApPENDIX G:

## SAMPLE MODMAN InPUT: OFFUTT



| 1 | 4 | 32 | 79 |
| :---: | :---: | :---: | :---: |
| 2 | 4 | 32 | 80 |
| 3 | 4 | 33 | 79 |
| 4 | 4 | 36 | 83 |
| 5 | 4 | 36 | 84 |
| 6 | 4 | 37 | 83 |
| 7 | 4 | 40 | 86 |
| 8 | 4 | 40 | 87 |
| 9 | 4 | 41 | 86 |
| 10 | 4 | 43 | 90 |
| 11 | 4 | 43 | 91 |
| 12 | 4 | 44 | 90 |
| 13 | 4 | 46 | 94 |
| 14 | 4 | 46 | 95 |
| 15 | 4 | 47 | 94 |
| 16 | 4 | 49 | 99 |
| 17 | 4 | 49 | 100 |
| 18 | 4 | 50 | 99 |
| 19 | 4 | 52 | 103 |
| 20 | 4 | 52 | 104 |
| 21 | 4 | 53 | 103 |
| 22 | 4 | 54 | 106 |
| 23 | 4 | 54 | 107 |
| 24 | 4 | 55 | 106 |
| 25 | 4 | 56 | 109 |
| 26 | 4 | 56 | 110 |
| 27 | 4 | 57 | 109 |
| 28 | 4 | 58 | 110 |
| 29 | 4 | 58 | 111 |
| 30 | 4 | 59 | 110 |
| 31 | 4 | 61 | 111 |
| 32 | 4 | 61 | 110 |
| 33 | 4 | 64 | 110 |
| 34 | 4 | 65 | 110 |
| 35 | 4 | 64 | 109 |
| 36 | 4 | 66 | 108 |
| 37 | 4 | 67 | 108 |
| 38 | 4 | 66 | 107 |
| 39 | 4 | 67 | 104 |
| 40 | 4 | 68 | 104 |
| 41 | 4 | 67 | 101 |
| 42 | 4 | 66 | 101 |
| 43 | 4 | 67 | 98 |
| 44 | 4 | 66 | 98 |
| 45 | 4 | 66 | 92 |
| 46 | 4 | 65 | 92 |
| 47 | 4 | 66 | 86 |
| 48 | 4 | 67 | 86 |
| 49 | 4 | 65 | 79 |
| 50 | 4 | 66 | 79 |
| 51 | 4 | 65 | 80 |
| 52 | 4 | 64 | 70 |
| 53 | 4 | 65 | 70 |
| 54 | 4 | 64 | 71 |
| 55 | 4 | 63 | 65 |
| 56 | 4 | 64 | 65 |
| 57 | 4 | 63 | 66 |
| 58 | 4 | 67 | 103 |
| 59 | 4 | 66 | 87 |

SET4: Head Limits
SET

| 4 |  |  | 31 | 32 |
| :--- | :--- | :--- | :--- | :--- |
|  | 1 | 1 | 41 | 42 |
|  | 3 | 1 | 43 | 4 |
|  | 1 | 45 | 46 |  |


| $0 . E+00$ | $1 \cdot E+20$ |
| :--- | :--- |
| $0 \cdot E+00$ | $1 \cdot E+20$ |
| $0 . E+00$ | $1 \cdot E+20$ |
| $0 . E+00$ | $1 \cdot E+20$ |

-10.00 1. $\mathrm{E}+20$

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|  | 2 | 1 | 1 | 3 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 3 | 1 | 4 | 5 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 4 | 1 | 4 | 6 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 5 | 1 | 7 | 8 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 6 | 1 | 7 | 9 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 7 | 1 | 10 | 11 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 8 | 1 | 10 | 12 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 9 | 1 | 13 | 14 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 10 | 1 | 13 | 15 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 11 | 1 | 16 | 17 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 12 | 1 | 16 | 18 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 13 | 1 | 19 | 20 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 14 | 1 | 19 | 21 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 15 | 1 | 22 | 23 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 16 | 1 | 22 | 24 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 17 | 1 | 25 | 26 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 18 | 1 | 25 | 27 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 19 | 1 | 28 | 29 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 20 | 1 | 28 | 30 | $0 . \mathrm{E}+00$ | 1. $\mathrm{E}+20$ |  |
|  | 21 | 1 | 33 | 35 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 22 | 1 | 33 | 34 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 23 | 1 | 36 | 38 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 24 | 1 | 36 | 37 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 25 | 1 | 49 | 51 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 26 | 1 | 49 | 50 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 27 | 1 | 52 | 54 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 28 | 1 | 52 | 53 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 29 | 1 | 55 | 57 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 30 | 1 | 55 | 56 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 31 | 1 | 39 | 58 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 32 | 1 | 39 | 40 | -10.00 | 1. $\mathrm{E}+20$ |  |
|  | 33 | 1 | 47 | 59 | 0.00 | 1. $\mathrm{E}+20$ |  |
|  | 34 | 1 | 47 | 48 | -10.00 | 1. $\mathrm{E}+20$ |  |
| SET7B: Velocity Limits |  |  |  |  |  |  |  |
| SET7C: Relative Gradient Limits17 |  |  |  |  |  |  |  |
|  | 1 | 2 | 1 | 1.00 |  |  |  |
|  | 2 | 4 | 3 | 1.00 |  |  |  |
|  | 3 | 6 | 5 | 1.00 |  |  |  |
|  | 4 | 8 | 7 | 1.00 |  |  |  |
|  | 5 | 10 | 9 | 1.00 |  |  |  |
|  | 6 | 12 | 11 | 1.00 |  |  |  |
|  | 7 | 14 | 13 | 1.00 |  |  |  |
|  | 8 | 16 | 15 | 1.00 |  |  |  |
|  | 9 | 18 | 17 | 1.20 |  |  |  |
|  | 10 | 20 | 19 | 1.43 |  |  |  |
|  | 11 | 21 | 22 | 0.58 |  |  |  |
|  | 12 | 23 | 24 | 1.00 |  |  |  |
|  | 13 | 25 | 26 | 2.14 |  |  |  |
|  | 14 | 27 | 28 | 2.14 |  |  |  |
|  | 15 | 29 | 30 | 2.14 |  |  |  |
|  | 16 | 31 | 32 | 5.67 |  |  |  |
|  | 17 | 33 | 34 | 5.67 |  |  |  |
| SET8: Balance Constraints14 |  |  |  |  |  |  |  |
|  | 1 | C |  | E | $0 . \mathrm{E}+00$ | 2 | */lf4-pw3 |
| 1 | 1 | 1.00 |  |  |  |  |  |
| 1 | 2 | -. 44 |  |  |  |  |  |
|  | 2 | C |  | E | $0 . \mathrm{E}+00$ | 2 | */lf4-pw4 |
| 1 | 3 | 1.00 |  |  |  |  |  |
| 1 | 4 | -. 49 |  |  |  |  |  |
|  | 3 | C |  | E | $0 . \mathrm{E}+00$ | 2 | */h2c-pw1 |
| 1 | 5 | 1.00 |  |  |  |  |  |
| 1 | 6 | -1.28 |  |  |  |  |  |
|  | 4 | C |  | E | $0 . \mathrm{E}+00$ | 2 | */h2c-core1 |
| 1 | 8 | 1.00 |  |  |  |  |  |
| 1 | 7 | -9.03 |  |  |  |  |  |
|  | 5 | C |  | E | $0 . \mathrm{E}+00$ | 2 | */h2c-core1 |
| 1 | 8 | 1.00 |  |  |  |  |  |
| 1 | 9 | -1.31 |  |  |  |  |  |
|  | 6 | C |  | E | $0 . E+00$ | 2 | */toe-new1 |



## Appendix H:

## Efficiently Making Modifications to MODMAN Formulations

Numerous hydraulic optimization formulations were solved with the MODMAN code as part of this demonstration project. However, each formulation did not require a separate execution of the MODMAN code. A MODMAN execution has the following major steps:
(1) execute MODMAN (mode 1) to create an MPS file (a linear or mixed-integer program);
(2) execute LINDO to solve the linear or mixed-integer program; and
(3) execute MODMAN (mode 2) to post-process the LINDO results.

In many cases, it is possible to slightly modify the hydraulic optimization formulation without re-executing MODMAN in mode 1. This can be accomplished by:
(1) modifying the MPS file with a text editor, prior to running LINDO; or
(2) modifying the linear or mixed-integer program directly within LINDO.

In many cases, LINDO results can be extracted manually, and there is no need to execute MODMAN in mode 2 (to post-process LINDO output).

For example, Section 4.4.2 discusses a series of mathematical optimal solutions for Kentucky, where the head limit at cells adjacent to the river is varied. The base formulation has an upper limit of 399.99 ft MSL assigned at 54 cells. To generate the mathematical optimal solutions associated with the other head limits, a text editor was used to modify the upper bounds on the appropriate variables in the MPS file. LINDO then solved the modified MPS file.

Another example is the generation of mathematical optimal solutions for related problems, where integer constraints are used to limit the number of wells selected. There is a specific constraint that has the following general form (see Section 3.1.3):

$$
\mathrm{I}_{1}+\mathrm{I}_{2}+\mathrm{I}_{3}+\mathrm{I}_{4}+\mathrm{I}_{5}+\mathrm{I}_{6} \mathrm{I}_{7}+\mathrm{I}_{8}+\mathrm{I}_{9} \leq 2
$$

The "right-hand side" of this constraint sets the limit on the number of active wells. This limit can easily be altered in the MPS file with a text editor, or altered directly within the LINDO software.

A full discussion of the structure of the MPS file, and potential complexities associated with modifying the MPS file (e.g., scaled well rates) is beyond the scope of this report. For more information, refer to the MODMAN User's Guide (Greenwald, 1998a).

## Appendix I:

## Sources of Information and References For Other Optimization Research and Application

The purpose of this appendix is to guide readers of this report to individuals or organizations that offer additional information on optimizations of groundwater systems. Although this is by no means a comprehensive reference section regarding optimization of groundwater systems, it should provide the reader with sufficient data to pursue additional information on a wide variety of subjects associated with optimization of groundwater systems.

A partial listing of individuals/organizations associated with optimization of groundwater systems is provided below:

| Name | Affiliation or Company | Address | Phone/Fax/Email |
| :---: | :---: | :---: | :---: |
| David <br> Ahlfeld | University of Massachusetts | Dept. of Civil and Env. Engineering <br> 139 Marston Hall <br> University of Massachusetts <br> Amherst, MA 01003 | Voice: (413) 545-2681 <br> Fax: (413) 545-2202 <br> ahlfeld@ecs.umass.edu |
| Paul <br> Barlow | U.S.G.S | 28 Lord Road <br> Marlborough, MA 01752 | Voice: (508) 490-5070 Fax: pbarlow@usgs.gov |
| Wes <br> Danskin | USGS Water <br> Resources | 5735 Kearney Villa Road, Suite 0 San Diego, CA 92123 | Voice: 619-637-6832 <br> Fax: 619-637-9201 <br> wdanskin@usgs.gov |
| David <br> Dougherty | Subterranean <br> Research, Inc. | P.O. Box 1121 <br> Burlington, VT 05402 | Voice: (802)-658-8878 <br> Fax: (802)-658-8878 <br> David.Dougherty@subterra.com |
| Steve <br> Gorelick | Stanford <br> University | Dept. of Geological and Env. Sciences Stanford University Stanford, CA 94305-2115 | Voice: (415) 725-2950 <br> Fax: (415) 723-1445 gorelick@geo.stanford.edu |
| Rob Greenwald | HSI GeoTrans, Inc. | 2 Paragon Way <br> Freehold, NJ 07726 | Voice: 732-409-0344 <br> Fax: 732-409-3020 <br> rgreenwald@hsigeotrans.com |
| George <br> Karatzas | Technical University of Crete | Dept. of Environmental Engineering Polytechneioupolis 73100 Chania Greece | Phone: (011-30-821) 37473 <br> Fax: (011-30-821) 37474 <br> karatzas@emba.uvm.edu |
| Ann <br> Mulligan | University of Massachusetts | Dept. of Civil and Env. Engineering 139 Marston Hall <br> University of Massachusetts Amherst, MA 01003 | Voice: (413) 545-2681 <br> Fax: (413) 545-2202 <br> mulligan@ecs.umass.edu |


| Name | Affiliation or Company | Address | Phone/Fax/Email |
| :---: | :---: | :---: | :---: |
| Daene <br> McKinney | University of Texas | Department of Civil Engineering Austin, TX 78712 | Voice: 512-471-8772 <br> Fax: 512-471-0072 <br> Daene@AOL.com |
| Tracy <br> Nishikawa | U.S.G.S. | 5735 Kearney Villa Road, Suite 0 San Diego, CA 92123 | Voice: 619-637-6848 <br> Fax: 619-637-9201 tnish@usgs.gov |
| David <br> Watkins | US Army Corps of Eng., Hydrologic Engineering Center | 609 Second Street Davis, CA 95616-4587 | Voice: 530-756-1104 <br> Fax: 530-756-8250 <br> david.w.watkins@usace.army.mil |
| Richard C. <br> Peralta | Utah State University | Building EC-216 <br> Utah State University Logan, UT 84322-4105 | Voice: 801-797-2786 <br> Fax: 801-797-1248 peralta@cc.usu.edu |
| George Pinder | University of Vermont | Dept. of Civil and Env. Engineering 371 Votey Building Burlington, VT 05405-0156 | Voice: 802-656-8697 <br> Fax: 802-656-8446 George.Pinder@uvm.edu |
| Eric <br> Reichard | U.S.G.S. | 5735 Kearney Villa Road, Suite 0 San Diego, CA 92123 | Voice: 619-637-6834 <br> Fax: 619-637-9201 <br> egreich@usgs.gov |
| Donna <br> Rizzo | Subterranean <br> Research, Inc. | P.O. Box 1121 <br> Burlington, VT 05402 | Voice: 802-658-8878 <br> Fax: 802-658-8878 <br> Donna.Rizzo@subterra.com |
| Christine Shoemaker | Cornell University | Civil Engineering Hollister Hall Ithaca, NY 14853 | Voice: 607-255-9233 <br> Fax: 607-255-9004 cas12@cornell.edu |
| Brian <br> Wagner | U.S.G.S, | Bldg 15, McKelvey Building 345 Middlefield Road, MS 409 Menlo Park, CA 94025 | Voice:650-329-4567 <br> Fax: <br> bjwagner@usgs.gov |
| Chunmiao <br> Zheng | University of Alabama | Department of Geology University of Alabama Tuscaloosa, AL 35487 | Voice: 205-348-0579 <br> Fax: 205-348-0818 czheng@wgs.geo.ua.edu |

As part of this project, information was solicited from select professionals involved in optimization code development for groundwater problems. The following pages provide brief summaries of codes and/or applications, provided by those professionals who responded:

## Code/Method: MODOFC (MODflow Optimal Flow Control) <br> Description By: David Ahlfeld, University of Massachusetts

Brief Description: MODOFC (MODflow Optimal Flow Control) is a FORTRAN computer program which determines optimal pumping solutions for groundwater flow control problems. MODOFC couples the USGS MODFLOW simulation program with optimization algorithms. The code can accommodate linear pumping costs, well installation costs, bounds on head and head difference, bounds on individual and net well pumping rates and bounds on total number of wells. MODFLOW features that can be accommodated include three-dimensional heterogeneous aquifers, confined or unconfined units, wells screened in single or multiple layers and single or multiple stress periods. MODOFC is designed to utilize existing MODFLOW96 input files along with a user-created file describing the hydraulic control problem. MODOFC converts the groundwater flow control problem into an optimization problem by the response matrix method. MODOFC contains a full implementation of the simplex algorithm. The simplex and branch and bound algorithms are used for mixed binary problems. Sequential linear programming is used for unconfined problems.

Application(s): An early version of MODOFC was used to design a groundwater pump and treat remediation system in coastal New Jersey. The aquifer was contaminated with a plume extending over several hundred acres and nearly 100 feet vertically. The site consisted of approximately 50 extraction wells, several recharge basins and pumped approximately 3 million gallons per day. The site was modeled with MODFLOW with five numerical layers and 35,000 grid cells. The results are presented in Ahlfeld et. al. (1995) and Pinder et. al. (1995).

## References:

Availability: MODOFC is available free of charge on the world wide web at "http://www.ecs.umass.edu/modofc/"

Point(s) of Contact: David Ahlfeld (see table at beginning of this Appendix).

| Code/Method: | MODFLIP |
| :---: | :---: |
| Description By: | David Dougherty, Subterranean Research, Inc. |
| Brief Description: | MODFLIP couples the popular MODFLOW groundwater simulation program with $\underline{\text { linear and mixed }}$ integer programming optimization [Fourer et al., 1993]. MODFLIP can be used to compute the optimal pumping strategies for groundwater management problem for which a reliable MODFLOW model exists, like other optimization programs described in this Appendix. Linear programming (LP) is limited in applicability to problems having linear (that is, proportionality) relations among cost, pumping rates, and all constraints. This approach can be applied, therefore, to groundwater flow in confined aquifers. If approximations are introduced, it can be applied in other cases that are weakly nonlinear, such as unconfined aquifers with small drawdowns. Mixed integer programming provides for fixed or one-time costs. The design of MODFLIPs mathematical optimization relies on a two-part objective function. The first is proportional to the amounts of pumping out of or into (extraction or injection) candidate wells. Through a linearization method, the energy costs (lift) can be included. The second part of the objective function is proportional to a binary (on-off, or one-zero) variable, which indicates whether a particular candidate well is selected or not. This term allows for costs including drilling, casing, and screen. Constraints on heads, head differences, and pumping rates are possible. In addition, the ratio of total injection to extraction can be constrained (e.g., to ensure that all extracted water is reinjected). Gorelick et al. [1989] provide a large number of two-dimensional examples to which linear programming is applicable; this software expands on their list by allowing fully 3-D flow conditions. |
| Application(s): | MODFLIP is applicable to steady flow optimization, linear programming, and linear mixed-binary programming problems. |
| References: | Fourer, R., D. M. Gay, B. W. Kernighan, Ampl: A Modeling Language for Mathematical Programming, Duxbury Press, Pacific Grove, CA, 1993. |
|  | Gorelick, S., R. A. Freeze, D. Donahue, and J. F. Keely, Groundwater Contamination: Optimal Capture and Containment, Lewis Publishers, 385 pp., 1989. |
|  | Subterranean Research, Inc., MODFLIP, A MODFLOW-based Program for Flow Optimization, http://www.subterra.com/publications/MODFLIP.pdf, 1999. |
| Availability: | Contact points of contact listed below. |

## Code/Method: Description By:

REMAX
Richard Peralta, Utah State University

Brief Description:
REMAX can compute optimal pumping strategies for any ground-water system for which you have a reliable simulation model. For simple dynamic stream-aquifer problems REMAX can also compute optimal conjunctive use strategies. Such a strategy includes optimal surface water diversion and ground-water pumping rates. REMAX can assure that implementing the optimal water management strategy will not cause unacceptable physical system responses. To do this the modeler specifies limits on acceptable responses. REMAX can constrain aquifer hydraulic heads, gradients, and flows. It can constrain streamflow in simple stream-aquifer management problems. For special situations REMAX has been adapted to constrain contaminant concentrations in ground water or surface water, or volumes of nonaqueous phase liquids (free product, residual, extracted). REMAX can address a wide range of volumetric, economic or environmental problems involving ground-water management. To do this it solves optimization problems having objective functions and constraints that are linear, nonlinear, integer or mixed integer. REMAX performs deterministic or stochastic, single- or multiobjective optimization. REMAX simulates using either standard numerical simulation models such as MODFLOW or response matrix (superposition) models that use influence coefficients derived via simulation models. REMAX employs response matrix methods adapted to accurately address nonlinear systems (unconfined aquifers). For special situations (often involving contaminant management), linear and nonlinear response surface methods are also used.

## Application(s): 1. Optimal Pumping Strategy to Capture TCE Plume at Southwest Base Boundary, Norton AFB

 (NAFB), California.TCE Plume was about 4 miles long and 1 mile wide. Site modeled using 3-layer MODFLOW model. Top layer was up to about 300 feet thick.Used REMAX Simulation/Optimization (S/O) model to optimize steady pumping. Initially assumed over 20 candidate wells, 40 gradient constraints in optimization problem. It was challenging because base boundary was irregular and all wells had to be on base. This was steady flow (hydraulic) optimization. Optimal pumping system design and strategy was built and implemented. It involved a total extraction of 2250 gpm ; total of 3 extraction wells and 8 injection wells. It saved about $20 \%$ ( $\$ 5.8 \mathrm{M}$ in present value) when compared with a design provided by a consulting firm that did not use $\mathrm{S} / \mathrm{O}$ modelling. Sensitivity analysis demonstrated the strategy should be valid even if hydraulic conductivity differed widely from assumed mean value (ie $60 \%$ underestimation .through $80 \%$ overestimation).2. Multiobjective Optimization: Maximizing Pumping for Water Supply versus Minimizing Pumping Needed for Plume Containment Subject to Lower Bound on Seepage from Aquifer to River (an anonymous site in the Northeast US). A contaminant plume existed under an industrial facility that had 3 wells and used some of the pumped water in industrial processes. Pumping from 3 upgradient public supply wells causes plume to be captured by those supply wells. MODFLOW was used to model the three-layer system. An anonymous contractor developed a steady pumping strategy using simulation model alone. REMAX was used for multiobjective linear steady flow (hydraulic) optimization. All scenarios involved Linear Programming. The first scenario was single objective: minimize total pumping needed to prevent the plume from moving to public wells, subject to constraints. The optimal pumping strategy required 40 percent less pumping than that developed by other contractor using only a simulation model. Later the municipality wanted to increase total pumping for water supply. This would require that the industry increase their total pumping to retain plume containment. However, the state water resources agency was concerned that the increases in pumping would dewater the nearby river too much. REMAX was used to develop the pareto optima solutions for this multiobjective problem.
3. Calibration of a Flow Model and Optimal Pumping Strategies to Capture a TCE Plume at Travis AFB (TAFB), California. TCE plume had migrated under a runway and emerged on the other side. It
was moving toward a stream that flowed toward and important wetland. Site modeled using 4-layer MODFLOW model, 5040 cells per layer. Plume exists in top three layers. REMAX was used to develop the minimum steady pumping needed from many candidate wells. It used many gradient constraints. This was steady flow optimization. Optimal pumping system design and strategy involved 5 extraction wells with pumping rates between 5 and 11 gpm . Total extraction is about 40 gpm .
4. Optimal Pumping Strategy to Contain a TCE Plume at March AFB (MAFB), California. TCE plume had crossed base boundaries and was under an urbanized area and was moving toward water supply wells. Site was modeled using a 4-layer SWIFT model. Contamination existed in multiple layers. REMAX was used to develop the minimum steady pumping needed from many candidate wells. It used many gradient constraints. This was steady flow (hydraulic) optimization.
5. Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Central Base Area, Norton AFB, California. TCE plume at a source area was to be remediated. MODFLOW and MT3D were used for a single layer system. Wells were already installed. Transient (two stress periods) transport optimization was used to develop maximum mass removal transient pumping strategies a specific planning horizon. Strategies were developed for a range of scenarios...differing in the maximum total pumping rate (200-400 gpm) and the wells that could be used. Enhanced REMAX was used. This showed the importance of applying optimization as early in the design process as possible. If one had to use existing wells and the same upper limit on total pumping, the optimal strategy was not much better than the existing strategy. If one could use different wells locations and the same total pumping, the amount of TCE mass removed could increase by about $20 \%$. Increasing total pumping permits increased mass removal.
6. Optimal Pumping Strategies to Maximize Dissolved TCE Extraction at Mather AFB, California. TCE plume at a source area was to be remediated. MODFLOW and MT3D were used to simulate flow and transport in a two layer system having 2184 cells in each layer. Wells were already installed. Transient (two stress periods) transport optimization was used to develop maximum mass removal for a specific planning horizon. Strategies were developed for a range of scenarios.. differing in the maximum total pumping rate and the wells that could be used. Enhanced REMAX was used. Using the existing wells and the same total pumping, over twenty percent increase in total mass removal is possible. Using alternative wells can increase mass removal. Raising upper limit on total pumping increases TCE mass removal.
7. Optimal Pumping Strategies for Cleanup and Containment of TCE and DCE Plumes Near Mission Drive, Wurtsmith Air Force Base (WAFM), Michigan. TCE and DCE plumes were projected to reach a stream. The goal is plume containment and cleanup (to specified concentration) within a planning horizon. MODFLOW and MT3D were the models used to represent this 3-layer system. First, genetic algorithm was used in nonlinear programming transport optimization to maximize mass removal subject to constraints. Strategies were developed for a range of total pumping rates being processed by the treatment plant. Objective was to maximize TCE mass removed subject to: (1) upper limit on final TCE and DCE aquifer concentrations; (2)upper limit on TCE concentration entering the treatment facility during any time step.; and (3)upper limit on total flow. Then the additional minimal pumping needed to achieve containment was determined using REMAX. Additional wells were added as needed. This was linear steady flow (hydraulic) optimization. Objective was to minimize total pumping subject to: (1) using the cleanup wells to the extent possible; and (2)containing the plume using hydraulic gradient constraints. Finally, optimal pumping strategies were developed for a range of treatment facility capacities.

References: Contact Richard Peralta

Availability: $\quad$ For sale (contact Richard Peralta)

Point(s) of Contact: Richard Peralta (see table at beginning of this Appendix).

## Code/Method: <br> Global Optimization Methods (Genetic Algorithms, Simulated Annealing, and Tabu Search) Description By: Chunmiao Zheng, University of Alabama

Brief Description: As part of our research efforts in the area of groundwater remediation design optimization in the last several years, we have developed a number of general-purpose flow and transport simulationoptimization software tools. These software tools combine the MODFLOW (McDonald and Harbaugh, 1988) and MT3D/MT3DMS (Zheng, 1990; Zheng and Wang, 1998) codes for flow and transport simulation with a general optimization package for formulating the most cost-effective groundwater management and remedial strategies under various physical, environmental and budgetary constraints. The optimization package is implemented with three global optimization methods, namely, genetic algorithms, simulated annealing and tabu search. The global optimization methods have the ability to identify the global or near-global optimum, are efficient in handling discrete decision variables such as well locations, and can be easily linked to any flow and transport simulation models for solving a wide range of field problems. They are also very easy to understand and simple to use.

Our global optimization based management tools are capable of determining time-varying pumping/injection rates and well locations for three-dimensional field-scale problems under very general conditions. The objective function of the optimization model can be highly nonlinear and complex. Most types of constraints that are commonly encountered in the field, such as prescribed hydraulic gradients, minimum drawdowns, and maximum concentration limits, can be readily incorporated. To account for the uncertainties in the groundwater flow and contaminant transport models, our software has a dual formulation to allow the user to perform automated parameter estimation given observed head and concentration data. Since our software does not require any changes to the input files prepared for MODFLOW and MT3D/MT3DMS, it can be used with any graphical user interfaces developed for MODFLOW and MT3D/MT3DMS, including Visual MODFLOW, DoD GMS, and Groundwater Vista.

The most significant limitation of the global optimization based management tools is their intensive computational requirements. To mitigate this problem, global optimization methods may be integrated with linear or nonlinear programming as we have recently demonstrated (Zheng and Wang, 1999). This integrated approach takes advantage of the fact that global optimization methods are most effective for dealing with discrete decision variables such as well locations while traditional programming methods may be more efficient for dealing with continuous decision variables such as pumping rates. Our preliminary work shows that it is possible to achieve dramatic reductions in runtime with the integrated approach.

## Application(s): Our simulation-optimization tools have been successfully applied to remediation design optimization

 problems at several field sites with complex hydrogeologic conditions. A typical example is presented by Wang and Zheng (1997) involving optimization of an existing pump-and-treat system at a gasoline terminal site in Granger, Indiana. Groundwater beneath and down-gradient of the site was found to contain dissolved compounds associated with petroleum hydrocarbons in extensive field investigations. Groundwater flow and solute transport models were developed in previous remedial investigations and feasibility studies to evaluate the various remedial alternatives at the site. A pump-and-treat system was already designed through the trial-and-error approach and implemented at the site.The optimization approach was applied to the same remediation design problem for comparison with the trial-and-error approach. Because the flow field was considered steady-state, and the fixed capital costs were negligible relative to the pumping and treatment costs, the objective function was simplified as minimizing the total pumping at eight existing wells subject to the constraint that the maximum
concentration level in the entire model must not exceed a specified value at a specific time. For comparison with the trial-and-error solution, the concentration limit for the optimization problem was set equal to the calculated maximum concentration at the end of the comparison period based on the pumping rates from the trial-and-error solution. The optimization solution reduces the total extraction of the trial-and-error solution by approximately 64 percent, demonstrating the significant economic benefits that may be derived from the use of the simulation-optimization models in remediation system designs.

## References: Glover, F. 1986. Future paths for integer programming and links to artificial intelligence. Comp. and

 Operations Res., 5, p. 533-549.McDonald, M.G. and A.W., Harbaugh. 1988. A Modular Three-Dimensional Finite-Difference Groundwater Flow Model. Techniques of Water Resources Investigations, Book 6, USGS.

McKinney, D.C. and M.-D. Lin. 1994. Genetic algorithms solution of groundwater management models, Water Resour. Res., 30(6), p. 1897-1906.

Rizzo, D.M., and D.E. Dougherty. 1996. Design optimization for multiple management period groundwater remediation, Water Resour. Res., 32(8), p. 2549-2561.

Wang, M. and C. Zheng. 1997. Optimal remediation policy selection under general conditions, Ground Water, 35(5), p. 757-764.

Wang, M. and C. Zheng. 1998. Application of genetic algorithms and simulated annealing in groundwater management: formulation and comparison, Journal of American Water Resources Association, vol. 34, no. 3, p. 519-530.

Zheng, C. 1990. MT3D, A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems. Report to the USEPA, 170 pp.

Zheng, C. and P.P. Wang. 1998. MT3DMS, A Modular Three-Dimensional Multispecies Transport Model, Technical Report, U.S. Army Engineer Waterways Experiment Station.

Zheng, C. and P.P. Wang. 1999. An integrated global and local optimization approach for remediation system design, Water Resour. Res., 35(1), p. 137-146.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: Chunmiao Zheng (see table at beginning of this Appendix).

Code/Method: Simulated Annealing
Description By: David Dougherty, Subterranean Research, Inc.

Brief Description: Simulated annealing (SA) is an optimization method that can be applied to any setting. It has been applied to confined aquifers, unconfined aquifers, soil vapor extraction, flow-only control, and solute transport-driven control with constraints ranging from simple to exceedingly complex. It is structured to make discrete decisions (e.g., select from discrete pumping rates at remediation wells), although this can be modified. It can handle multiple management periods (sequences of operating schedules). SA is very well suited to difficult and large optimization problems, and performs poorly on small linear problems; it is therefore a perfect companion to LP. Like the outer approximation method, SA does not require a feasible initial problem to start, unlike many nonlinear (and linear) optimization methods. If there is no feasible solution to the problem, SA will provide "good" (though infeasible) solutions. When naively applied, SA can require enormous computing resources and time, while in experienced hands and when applied to appropriate problems the method is competitive with any other.

Application(s): Simulated annealing (SA) and related methods (e.g., elements of tabu search) were introduced into the groundwater literature by Dougherty and Marryott [1991]. At a central California site, the method was applied in a post mortem approach to determine if cleanup could have been accomplished with less expense. Marryott, Dougherty, and Stollar [1991] report that a $40 \%$ reduction in pumping rates could have been achieved. Groundwater simulations used an engineering model developed by LLNL that was not modified for the optimization process. The method has been applied to a solvent plume at Lawrence Livermore National Laboratory during the design phase; SA selected clever locations and operating schedules, and cost reductions in the tens of millions of dollars were identified [Rizzo and Dougherty, 1996]. SA has also been applied to a soil vapor extraction application [Sacks, Dougherty, and Guarnaccia, 1994]. To our knowledge, Subterranean Research, Inc. personnel have conducted the only applications of SA to field-scale problems.

References: Dougherty, D. E., and R. A. Marrott, "Optimal groundwater management, 1. Simulated annealing", Water Resources Research, 27(10), 2493-2508, 1991.

Marryott, R. A., D. E. Dougherty, and R. L. Stollar, "Optimal groundwater management, 2 Application of simulated annealing to a field-scale contamination site", Water Resources Research, 29(4), 847860, 1993.

Rizzo, D. M., and D. E. Dougherty, "Design optimization for multiple management period groundwater remediation", Water Resources Research, 32(8), 2549-2561, 1996.

Sacks, R. L., D. E. Dougherty, and J. F. Guarnaccia, "The design of SVE remediation systems using simulated annealing", 1994 Groundwater Modeling Conference, Fort Collins, CO, August 10-12, 1994.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: David Dougherty or Donna Rizzo (see table at beginning of this Appendix).

## Code/Method: Augmented Outer Approximation

Description By: David Dougherty, Subterranean Research, Inc.

Brief Description: Augmented Outer Approximation can be applied to containment and cleanup groundwater quality problems, as well as other water resources problems. Like the other methods described in this Appendix, a suitable and reliable aquifer simulation model is available. Outer approximation has been combined with the MODFLOW, MT3DMS, and SUTRA simulation models, for example.

The outer approximation method is a cutting plane optimization method designed originally for concave objectives (minimization) and convex constraints. Karatzas (see listing in this Appendix or the Karatzas and Pinder [1996] paper) describes extensions that accommodate nonconvex constraints, which occur in transport and other nonlinear optimization problems.

To solve larger problems faster and more effectively, Subterranean Research, Inc. has augmented outer approximation algorithms for groundwater problems in several ways. Among these are the following:

- A completely new data structure has been implemented, resulting in substantial speedups.
- New nonlinear algorithms adapt to nonconvex problems and a new "cutting depth" strategy.
- Completely new pivoting method for generating hyperplanes and associated data structures.
- Innovative method for subspace projection of optimization problem, resulting in substantially improved efficiency.

Application(s): Karatzas (see listing in this Appendix) cites several applications of the outer approximation method.
Subterranean Research, Inc. has conducted a range of test applications involving both synthetic and real sites.
References: $\quad$ Karatzas, G. P., and G. F. Pinder, "The solution of groundwater quality management problems have
non-convex feasible region using a cutting plane optimization technique", Water Resources Research,
vol. 32, no.4, 1091-1100, 1996.

Availability: Contact "points of contact" listed below.

Point(s) of Contact: David Dougherty or Donna Rizzo (see table at beginning of this Appendix).

Code/Method:
Description By:

The Outer Approximation Method
George Karatzas, Technical University of Crete

Brief Description: The Outer Approximation method is a cutting plane technique for the minimization of a concave function over a compact set of constraints that can have a convex or non-convex behavior. The basic concept of the method is that the minimum of a concave function occurs at one of the most "outer" points of the feasible region. The concept of the methodology is describe as follows: Initially, the feasible region is approximated by an enclosing polytope, which is defined by a set of vertices. Then, the vertex that minimizes the objective function is determined. If the vertex belongs to the feasible region this is the optimal solution, if not a cutting plane is introduced to eliminate part of the infeasible region and create a new enclosing polytope that is a "better" approximation of the feasible region. A new set of vertices is determined and the process is repeated until the optimal Solution is obtained. Depending on the behavior of the feasible region, convex or concave, a different approach is applied to determine the equation of the cutting plane. The method guarantees a global optimal solution. The Outer Approximation Method has the potential to solve groundwater management problems related to hydraulic gradient control and/or mass transport optimization problems. Additional features of the method are:

- It incorporates the well installation cost.
- It can incorporate treatment plant design (under development).
- It can handle combination of hydraulic gradient and concentration constraints.
- For small to average problems it can handle multi-period design problems.
- It can incorporate uncertainty (under development).


## Application(s):

The Woburn aquifer in Massachusetts. A remediation scheme using the developed Outer Approximation algorithm in combination with the 2-D numerical simulator, GW2SEN.
(2) The Lawrence Livermore National Laboratory Site in California. An optimal design using the Outer Approximation Algorithm in combination with a 2-D numerical simulation, SUTRA, and a 3-D numerical simulator, PTC (Princeton Transport Code).
(3) The U.S. Air Force Plant number 44, Tuscon, Arizona. Preliminary studies on the site, testing the existing pump-and-treat remediation scheme and propose and optimal remediation scheme using the Outer Approximation algorithm and a 3-D numerical simulator, PTC.

References: Karatzas, G. P., and G. F. Pinder, "Groundwater Management Using Numerical Simulation and the Outer Approximation Method for Global Optimization", Water Resources Research, vol. 29, no. 10, 3371-3378, 1993.
Karatzas, G. P., and G. F. Pinder, "The Solution of Groundwater Quality Management Problems with a Non-convex Feasible Region Using a Cutting Plane Optimization Technique", Water Resources Research, vol. 32, no. 4, 1091-1100, 1996.
Karatzas, G. P., A. A. Spiliotopoulos, and G. F. Pinder, "A Multi-period Approach for the Solution of Groundwater Management Problems using the Outer Approximation Method", Proceedings of the North American Water and Environment Congress '96, American Society of Civil Engineers, CDROM, 1996.

Availability: $\quad$ Code not in public domain, not for sale.

Point(s) of Contact: George Karatzas (see table at beginning of this Appendix).

