

REMAX

Simulation/Optimization Model for Management
of Stream/Aquifer Systems Using the
Response Matrix and
Related Methods

Version 2.70
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CONFIDENTIAL DRAFT

User's Manual

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Note

This software is more completely known as US/REMAX. In this manual, the acronym REMAX is used for brevity.

BRIEF CONTENTS

REMAX Manual Main Body	
1. Introduction	1
2. Hardware and Software Requirements	21
3. Installation	23
4. Overview	25
5. Tutorial	27
6. Example problems	33
7. How to benefit from REMAX	39
Appendix A. Trouble Shooting	A-1
Appendix B. Background for formulating an optimization problem using REMAX	B-1
Appendix C. Applying REMAX to Your Study Area	C-1
Appendix D. File formats	D-1
Appendix E. Example Problem EX1 - Regional Sustained Yield Planning . . .	E-1
Appendix F. Example Problem EX2 - Conjunctive Use	F-1
Appendix G. Example Problem EX3 - Plume Management	G-1
Appendix H. Bibliography	H-1
Appendix I. Terminology, Acronyms, and Symbols	I-1
Appendix J. REMAX Utilities	J-1
Appendix K. Case History (Multiobjective Optimization: maximizing municipal pumping, while controlling a plume and preventing unacceptable river dewatering.) and Pareto Optimum development	K-1

TABLE OF CONTENTS

REMAX Manual Main Body

1. Introduction	1
Purpose of this document	1
Why use a simulation/optimization model	2
Introduction and simple application of linear systems theory in groundwater management	2
A simple manually-solved groundwater management problem	4
A brief comparison between common simulation and S/O models	8
Purpose and features of REMAX	11
Objective Function Types Available in REMAX	14
Constraints in REMAX	16
Unique Features of REMAX version 2.70	17
Assumptions and limitations of REMAX	19
2. Hardware and Software Requirements	21
Hardware requirements	21
Software requirements	21
3. Installation	23
4. Overview	25
5. Tutorial	27
6. Example problems	33
EX1 - Regional Planning	34
EX2 - Conjunctive Use	36
EX3 - Plume Management	37
7. How to benefit from REMAX	39

Appendix A. Trouble Shooting

A.1. System errors	A-1
A.2. REMAX error messages	A-4

Appendix B. Background for formulating an optimization problem using REMAX

B.1. Introduction	B-1
B.2. Describing system response to hydraulic stresses	B-1
B.3. Objective function options	B-5
B.3.1. Linear objective	B-5
B.3.2. Quadratic objective.	B-7
B.3.3. Integer installation costs objective	B-8

B.3.4. Goal programming objective penalizing squared deviations	B-8
B.3.5. Goal programming objective penalizing absolute deviations	B-9
B.3.6. Goal programming objective penalizing maximum absolute deviation	B-10
B.3.7. Minimax objective	B-11
B.3.8. Maximin objective	B-11
B.4. Overview of possible constraints and bounds	B-13
B.5. Bounds on objective values	B-17
B.6. Bounds on decision variables	B-18
B.7. Bounds on aquifer potentiometric head	B-18
B.8. Constraints on aquifer head difference, hydraulic gradient, seepage velocity and contaminant velocity	B-19
B.9. Bounds on drain, river, and stream state variables and conditions	B-21
B.10. Bounds on nonlinear variables	B-25
B.11. Bounds on surface water contaminant concentration	B-28
B.12. Constraints on sums of decision variables, relations between decision variables, and relations between sums of decision variables	B-29
B.13. Review and summary	B-33
 Appendix C. Applying REMAX to Your Study Area	
C.1. Overview of the Simulation/Optimization Modelling Process	C-1
C.2. Relation of this manual to the S/O modelling process	C-3
C.3. Developing a preliminary optimal strategy for your study area	C-5
Activity 4, computing system response to nonoptimal (no-new-action) management	C-5
Activity 7, defining the optimization problem verbally	C-6
Activity 8, selecting the objective function, bounds and constraint equations	C-7
Activity 9, organizing and entering data input for REMAX	C-9
General instructions	C-9
Brief instructions for preparing REMAX.DAT, CONTROL.DAT, BOUNDS.DAT and OBJECTIV.DAT	C-10
Activity 10, Running the S/O model and calculating an optimal strategy	C-14
Activity 11, Evaluating system response to management	C-14

C.4. Closure	C-16
Appendix D. File formats	
D.00. Background	D-1
Overview of input files	D-1
Overview of output files	D-2
Terminology and Conventions	D-3
Using MODFLOW data files within REMAX	D-5
D1.0. Array input	D-8
D1.1. Basic Package	D-10
D1.2. Block-Centered Flow (BCF3) Package	D-13
D1.3. Well Package	D-16
D1.4. Drain Package	D-17
D1.5. River Package	D-18
D1.6. Evapotranspiration Package	D-19
D1.7. Transient Leakage Package	D-20
D1.8. General-Head Boundary Package	D-21
D1.9. Recharge Package	D-22
D1.10. Strongly Implicit Procedure Package	D-23
D1.11. Direct Solution Package	D-24
D1.12. Slice-Successive Overrelaxation Package	D-26
D1.13. Output Control Package	D-27
D1.14. Preconditioned Conjugate Gradient (PCG2) Package	D-29
D1.15. Generalized Finite Difference Package	D-31
D1.16. Horizontal Flow Barrier (HFB) Package	D-33
D1.17. Streamflow-routing Package	D-34
D1.18. Interbed Storage (IBS) Package	D-37
D1.19. Time-Variant Specified Head Package	D-40
D1.20. Reservoir Package	D-41
D2.1. Manageable Stimuli Locations File	D-43
D2.2. Control Groups File	D-46
D2.3. Bounds and Constraints File	D-51
D2.4. Objective Function File	D-57
D2.5. Nonlinear Constraints File (WW.DAT)	D-63
D2.6. Surface Water Quality Control Definition File(SQUAL.DAT)	D-77
D2.7. Optimal Strategy Analysis File (ANALYSIS.DAT)	D-81
D3.1. LOG Files	D-83
D3.2. Influence Coefficient Files Produced by REMAX	D-84
D3.3. Optimization Output File (REMAX.OUT)	D-86
D3.4. Optimal Strategy Analysis Output File (ANALYSIS.OUT)	D-94

Appendix E. Example Problem EX1 - Regional Sustained Yield Planning	
E.1. Description	E-1
E.2. Input data files	E-6
E.3. Results	E-23
Appendix F. Example Problem EX2 - Conjunctive Use	
F.1. Description	F-1
Problem Formulation	F-3
F.2. Input for simulation	F-7
F.3. Application and Results	F-25
Appendix G. Example Problem EX3 - Plume Management	
G.1. Description	G-1
G.2. Input data files	G-7
G.3. Results	G-26
Appendix H. Bibliography	H-1
Appendix I. Terminology, Acronyms, and Symbols	I-1
I.1. Terminology and Acronyms	I-1
I.2. Symbols	I-3
Appendix J. REMAX Utilities	J-1
J.1. The Configuration Utility (CONFIGRX)	J-1
J.2. The Multiple-Realizations Utility (STACK)	J-3
J.3. The MT3D Utility (AUTOMT3D)	J-4
J.3.1. Input Data File (AUTOMT3D.DAT)	J-5
J.3.2. Output File Format (OUT.?)	J-7
J.3.3. Sample Input and Output Files	J-8
Appendix K. Case History	
(Multiobjective Optimization: maximizing municipal pumping, while controlling a plume and preventing unacceptable river dewatering.) and Pareto Optimum development	
K.1. Description	K-1
K.1.1. Introduction	K-1
K.1.2. Study area description and situation	K-1

K.2. Developing optimal pumping strategies	K-4
K.2.1. Developing a pumping strategy for the initial situation via common practice (Scenario 1 ^{non})	K-4
K.2.2. Developing, computing and verifying optimal pumping strategy for the initial situation via USA/REMAX (Scenario 1)	K-4
K.2.3. Developing optimal pumping strategy without placing a lower bound on industrial pumping (Scenario 2)	K-6
K.2.4. Developing optimal pumping strategy which maximizes municipal pumping while minimizing industrial pumping needed to control plume migration and preventing unacceptable river dewatering (Scenario 3)	K-6
K.2.5. Developing alternative pumping strategies	K-7
K.3. Two techniques of Pareto Optimum development in multiobjective optimization	K-11
K.3.1. Introduction	K-11
K.3.2. Weighting approach	K-11
K.3.2.1. Model	K-11
K.3.2.2. Procedure for developing the Pareto Optimum	K-11
K.3.3. E-Constraint method	K-12
K.3.3.1. Models	K-12
K.3.3.2. Procedure for developing the Pareto Optimum	K-12

LIST OF TABLES

Table 1.	Partial comparison between inputs and outputs of Simulation and Simulation/Optimization (S/O) models	10
Table B-1.	Signs of weighting coefficients needed to achieve specified management goals when MODFLOW is used (for objective functions which minimize)	B-7
Table B-2.	Indexing and numbers of variables and equations used in constraints	B-16
Table D-1.	OBJ values for some objective types	D-61
Table D-2.	Examples of Objective Types	D-62
Table F-1.	Stream inflow rates	F-3
Table F-2.	Summary of the scenarios	F-26
Table G-1.	Summary of Scenario Assumptions and Results	G-28
Table K-1.	Scenario results	K-4

LIST OF FIGURES

Figure 1.	Graphical representation of the simple groundwater optimization problem	6
Figure C-1.	REMAX conceptual overview	C-15
Figure E-1.	Map of study area for regional planning problem EX1	E-2
Figure F-1.	Map of the study area for conjunctive use problem EX2	F-2
Figure F-2.	Distorted map showing the segments and reaches used in the STR package data	F-6
Figure G-1.	Map showing locations of potential pumping, \hat{a} , and head-difference constraints, \hat{u}	G-3
Figure G-2.	One realization of the hydraulic conductivity of layer 1 (This realization is used for Scenarios 1 and 7-10)	G-4
Figure K-1.	(a) Finite-difference grid for the area (b) well locations and locations of head difference constraints imposed in Scenarios 1-3	K-3
Figure K-2.	Optimal pumping strategy for Scenario 1, Cycle 2	K-9
Figure K-3.	Relation between total pumping from municipal wells and total pumping from industrial wells	K-10
Figure K-4.	Weighting method	K-12
Figure K-5.	E-Constraint method	K-13

LIST OF WORKSHEETS

WORKSHEET C-1. Checking problem size restrictions	C-8
WORKSHEET C-2. Input files and dataitems (Appendix D) required to describe desired optimization problem equations (Appendix B)	C-11
WORKSHEET C-3. Input data organization (Appendix D) required to address desired optimization problem equations (Appendix B)	C-12

■ End of Table of Contents ■

**US/REMAX (VERSION 2.70): SOFTWARE FOR OPTIMIZING MANAGEMENT OF
STREAM/AQUIFER SYSTEMS USING THE RESPONSE MATRIX AND RELATED METHODS**

Richard C. Peralta and Alaa H. Aly¹

ABSTRACT: US/REMAX is designed to assist water managers in developing optimal groundwater and/or surface water strategies for a wide range of management problems. US/REMAX uses the response matrix method, which assumes that physical system response to stimuli is linear. However, US/REMAX can also address nonlinear systems via cycling. In one application, a strategy computed using US/REMAX required 40% less pumping than one obtained via a normal simulation model. US/REMAX also easily computes tradeoffs for multiobjective problems.
KEY TERMS: simulation/optimization model, conjunctive water management, groundwater, contamination, optimization.

INTRODUCTION

As competition for water resources intensifies, it becomes increasingly important to improve coordinated management of water and land resources. Water quality considerations add to analysis complexity. The ability to predict the effects of management practices on surface and groundwater flow and transport is important. Also needed is the ability to develop optimal management strategies for increasingly complex problems.

Currently, several well-documented, verified, and accepted computer models for simulating flow or transport in groundwater and surface water resources are available. These simulation (S) models can be used to guide management decisions. The modeler usually assumes several management strategies and uses the model to predict the consequences of implementing each of these strategies. Since there is generally an infinite number of strategies for a situation, the chance that the modeler assumes the absolutely best strategy is not great.

On the other hand, a Simulation/Optimization (S/O) model can compute the best management strategy directly. The modeler defines the management goal(s), restrictions on system response to the strategy. The S/O model finds the management strategy which is best for the posed management scenario. In the following sections, we present the capabilities of an S/O model (US/REMAX, version 2.70) and describe its features. Future model versions will have additional features.

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PURPOSE AND GENERAL FEATURES OF US/REMAX

As detailed in the user's manual (Peralta and Aly, 1993), US/REMAX assists water managers in developing and selecting optimal groundwater pumping (extraction and injection) and conjunctive water management strategies for a wide range of management problems. US/REMAX computes optimal pumping and diversion rates and resulting physical system responses using the Response Matrix Method. US/REMAX combines groundwater and open channel flow simulation with operations research optimization capabilities. Essentially, it performs three major activities:

- Simulation of system response to current (or nonoptimal) management and development of influence coefficients describing system response to unit hydraulic stimuli. In US/REMAX, this is referred to as **SIMULATION**.
- Selection of influence coefficients for specified control locations for the user-specified problem. This is referred to as **PRE-OPTIMIZATION**.
- Formulation of operations research optimization problem and computation of optimal pumping, diversion, and conjunctive water use strategies. This is referred to as **OPTIMIZATION**.

Depending on the weights used in the objective function of the optimization model, one can either minimize or maximize water pumped (from groundwater aquifers), or diverted (from surface streams), or pumped and diverted. Weighting coefficients can be used to emphasize pumping from individual (or groups of) potential pumping or diversion locations. Weighting coefficients can also be used as cost coefficients for linear or nonlinear economic optimization. Other objective functions can incorporate installation costs of wells and/or stream diversions, goal programming, and many other options.

US/REMAX (version 2.70) can specify the following for inclusion within the optimization problem (version 2.00 lacks items 2e, 10, 11, 12):

- 1) Potential locations for groundwater pumping and stream water diversion;
- 2) Locations at which any of the following will be bounded,
 - a) aquifer head
 - b) river- or stream-aquifer interflow in a reach or group of reaches
 - c) stream stage
 - d) outflow from a stream reach
 - e) other variables that can be described using a functional relation (linear or nonlinear) to pumping and/or diversion rates.
- 3) Locations between which head difference, hydraulic gradient, groundwater flow (or contaminant) velocity will be constrained;
- 4) Upper and lower bounds on groundwater pumping, stream water diversion, aquifer potentiometric head, head difference, gradient, groundwater velocity, groundwater contaminant velocity, river-aquifer interflow, stream stage, and stream outflow;
- 5) Upper and lower limits on sums of groundwater pumping, sums of stream water diversion, sums of pumping plus diversion, or sums of river-aquifer interflow (for all cells together or for groups of cells);
- 6) Monotonicity of pumping and/or diversion rates with time (increasing or decreasing)
- 7) Ratio between total groundwater extraction from and injection to the aquifer.
- 8) Effect of hydraulic stimuli on head just outside the casing of a pumping well.

- 9) Lower and upper limits on number of wells, stream diversions, or both.
- 10) Goals involving heads or virtually any other variable. US/REMAX uses goal programming to compute a strategy that will achieve the stated goals to the extent physically possible. Goal programming involves applying a penalty to goal non-achievement within the objective function. Absolute value and quadratic penalty functions are available. The user can also assign different weights for over- and under-achievement of the prescribed goals.
- 11) Integer programming enables users to specify lower and upper bounds on the "number" of wells and/or stream diversions. It also enables users to incorporate installation costs of wells and stream diversions into the objective function.
- 12) Nonlinear constraints: This option allows users to constrain (or use goal programming for) variables that can be described using a functional relation to pumping and/or diversion rates. The nonlinear variables can represent concentration of a contaminant in the groundwater aquifer, mass of contaminant extracted via an extraction well, free oil volume, and/or residual oil volume (for a problem involving LNAPL contamination).

US/REMAX requires input data concerning the physical system and stresses not subject to optimization. These are entered in the same format as is used by MODFLOW (McDonald and Harbaugh, 1988) and STR (Prudic, 1989). In addition, US/REMAX needs data concerning management goals for formulating the management problem.

Once data have been entered concerning the management goal, management constraints, and the physical system, the following occurs. US/REMAX computes nonoptimal head changes resulting from known (unit) stresses. Then it calculates influence coefficients describing system response to unit hydraulic stimuli (groundwater pumping or surface-water diversion). The modeler specifies all potential locations of optimizable stimuli and locations at which heads, gradients or velocities might be constrained within the optimization problem. The model organizes the optimization problem and then submits it to an optimization algorithm for solution. The optimization module then calculates an optimal water use strategy (consisting of pumping and diversion rates).

CONSTRAINTS AND BOUNDS ON DECISION AND STATE VARIABLES

Constraints refer to restrictions on decision variables or system responses to implementing the optimal management strategy. Upper or lower limits on individual decision or state variables are also commonly termed bounds. These bounds are upper and lower limits on variables about which managers commonly must make decisions. Numerical values of the bounds can vary with cell, group and time. Available constraints are listed below.

- 1) decision variables
 - groundwater pumping (withdrawal or recharge) rates
 - surface water diversion rates
- 2) aquifer state variables and conditions
 - potentiometric surface elevation
 - potentiometric surface head difference, hydraulic gradient, groundwater velocity or contaminant transport velocity between a pair of locations (any two points located in any two layers) (These are termed HGV constraints.)

- 3) river or stream state variables²
 - river- or stream-aquifer interflow
 - sum of river- or stream-aquifer interflows (for specified groups of cells)
 - stream flow rate
 - stream stage
- 4) sums of decision variables, and relations between decision variables and their sums
 - sum of groundwater extraction rates, diversion rates, and extraction plus diversion (for specified groups of cells)
 - relative change in decision variable values with time (monotonicity)
 - relation between total extraction and total injection

When formulating the bounds, groundwater extraction is negative in sign; groundwater recharge and river water diversion are positive. Thus, sample lower and upper bounds on groundwater extraction might be -10 and 0, respectively. Lower and upper bounds on injection at a cell might be 0 and 15, respectively.

Lower and upper bounds can be placed on the sums of pumping, diversion or pumping plus diversion in specified groups of cells, in each time step. If such a bound represents the minimum total rate of water that must be provided, it might be termed a demand constraint (and be based on current or historic water demand). If a bound represents the maximum total rate of water that can be provided, it might be termed a capacity constraint (and be based upon the maximum water that can feasibly be used, conveyed or distributed)

Long term planners and water users sometimes wish to assure that future pumping does not change erratically with time. In other words, that legally permitted pumping does not increase in one stress period (consisting of several years) and decrease in the next period. Thus, they might wish to assure that pumping is never less in one period than in a previous period. This goal can be achieved through monotonicity constraints applied to pumping or diversion. Depending on user preference, pumping and/or diversion can be forced to monotonically increase or decrease with stress period. Alternatively, pumping or diversion can be permitted to change freely with stress period.

ASSUMPTIONS AND LIMITATIONS OF US/REMAX

US/REMAX utilizes linear systems theory and superposition to compute an optimal pumping strategy. This involves computing system response to unit stimuli before optimization. During optimization, multiplicative and additive properties are used to represent system response to optimal stimuli. This is completely appropriate for confined aquifers because they are linear.

However, flows and head response to stimuli in stream-aquifer systems are sometimes nonlinear or piecewise linear. An example nonlinear process is flow in an unconfined aquifer in which head changes significantly affect transmissivity. MODFLOW treats that as a linear process, but changes transmissivity with each iterative solution of the flow equation. Processes represented as piecewise linear in MODFLOW include: stream-aquifer interflow, evapotranspiration, flow from drains, and vertical flow between layers.

A common rule of thumb is to assume that horizontal groundwater flow is linear as long as there is no more than a 10 percent change in transmissivity with time (Reilly et al, 1987). That generally results in less than 5 percent error in predicted head changes. However, one can reduce

² The term 'river' is used when MODFLOW's river package is utilized to develop influence coefficients. The term 'stream' is used when the STR package is utilized to develop influence coefficients. Diversion can be considered only when the STR package is used.

that error to much less than 5 percent by cycling. Cycling involves replacing the unit stimuli with the time average optimal pumping or diversion rates (or larger stimuli) and repeating the optimization (Gharbi and Peralta, 1994; Peralta and Kowalski, 1988). Through cycling one can satisfactorily compute optimal strategies for unconfined aquifers. The same process can be used to help address the piecewise linear processes listed above.

US/REMAX can optimize management of systems modelable using MODFLOW with or without the additional STR module. Systems modeled with STR are more nonlinear than those handled by MODFLOW alone. For example, STR uses the nonlinear Manning Equation to describe stream stage resulting from a particular stream flow. Thus, a particular influence coefficient describing the effect of a stimulus on stream stage might be valid only for a small range of conditions. Again, this nonlinearity can be addressed somewhat by cycling. Stream stage can also be controlled using nonlinear constraints in US/REMAX.

In summary, US/REMAX is completely and readily applicable to linear systems. When addressing nonlinear systems, accuracy is enhanced by cycling. When determining whether or how much to cycle one can consider how well the simulation model is calibrated to the study area and how well the aquifer is characterized. US/REMAX has the option of automatic cycling.

APPLICATION

In this section we discuss a multiobjective case history that combines concern about groundwater quality, public water supply and river depletion (a more detailed discussion of the problem can be found in Appendix K of the US/REMAX User's Manual, Peralta and Aly 1993). First, the study area and problem are described. Second, the steady-state pumping strategy developed by a consultant using MODFLOW is presented. Third, the problem is posed for solution via optimization, US/REMAX is applied, and an optimal strategy is computed. Then, the system response to implementing the optimal strategy is verified using simulation. Finally, variations in the management goals are assumed and new optimal strategies are developed. Computed optimal strategies are compared.

The study area (Figure 1), consisting primarily of glacial outwash, is about 1.9 by 1.8 miles in size and is discretized into 36 rows and 34 columns. The length of the cells ranges from 78.2 ft to 1980.2 ft. The width of the cells ranges from 138.4 ft to 1138.5 ft. The area is bounded on the west and east by impermeable material. There is fixed inflow from the north. The hydraulic gradient generally runs from north to south, paralleling flow in a river. The southern boundary consists of river cells.

Aquifer parameters were calibrated by a consultant. The unconfined aquifer is represented by three layers. Near the plume and the wells, the horizontal hydraulic conductivity is 600 ft/day for layers 1-3 (layer 1 is uppermost). Layer saturated thicknesses are about 22, 40 and 160 ft, respectively. Recharge due to rainfall is 0.027 ft/d.

A contaminant plume exists in the vicinity of an industrial facility. Unless influenced by groundwater pumping, the plume would migrate southward. Using 3 wells (referred to as industrial wells), that facility pumps and uses the underlying contaminated water. A municipality to the northeast of the facility also pumps from three wells. Total municipal pumping is 315,350 ft³/d. Municipal pumping causes the contaminated water to flow toward the northeast, unless the industrial wells pump significantly.

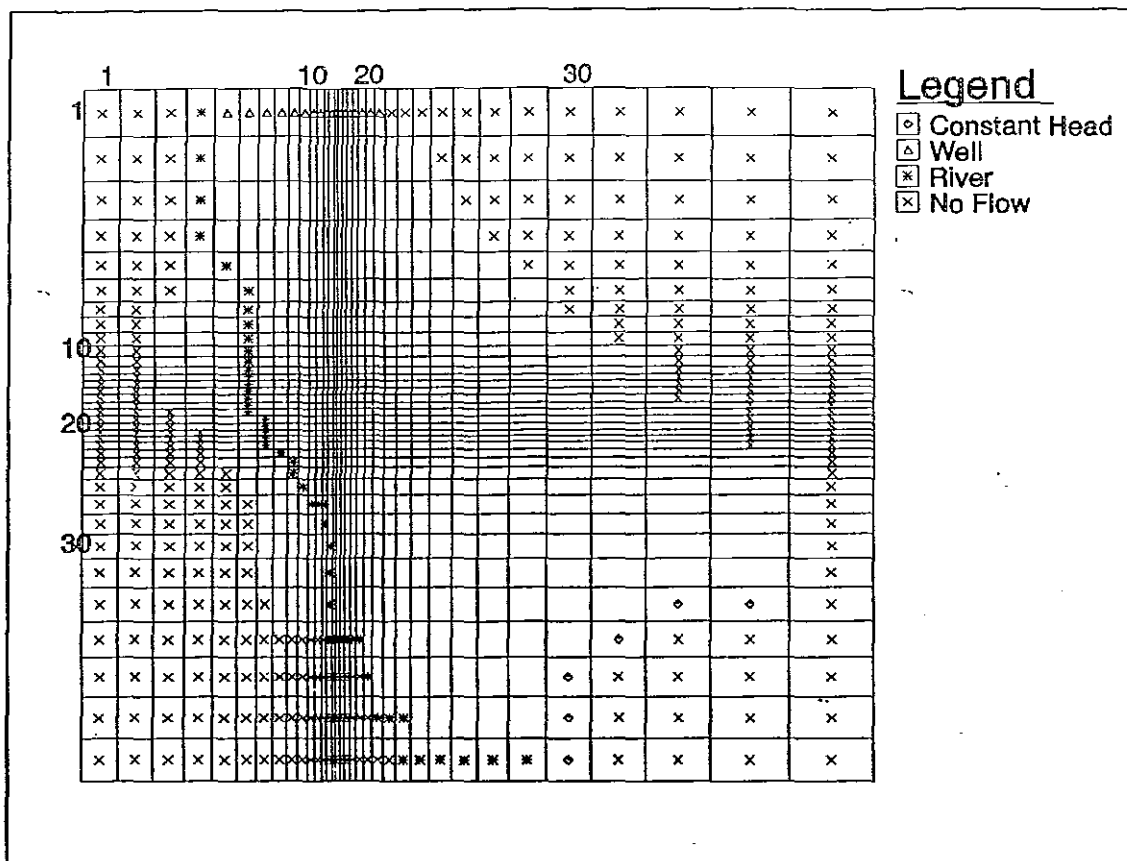


FIGURE 1. Study area; grid and boundary conditions.

Before US/REMAX was available, a consultant was asked to determine how much contaminated water must be pumped to keep the plume from reaching the public supply wells. The consultant developed a pumping strategy through repetitive simulations. For the next few years, the facility pumped at the recommended rate. Although it was not a consideration initially, a water supply agency then expressed concern about river flow depletion caused by the pumping. Another consideration is that the municipality might wish to increase pumping for public use--which will also cause river depletion. Accordingly, the consultant wanted to know how the pumping strategy could be revised to satisfy the disparate and conflicting goals. To do so, we used US/REMAX.

Below are presented (Table 1) and discussed the initial consultant solution (Scenario 1^{non}), the optimal solution to the same situation (Scenario 1), and optimal solutions to alternative management scenarios.

After calibrating MODFLOW, the consultant tested different combinations of pumping at the three industrial facility wells. Since the facility uses 267,380 ft³/d (2 mgd) in its processing, the consultant tried to develop a pumping strategy that would require as little excess pumping as possible, while making sure that there would be a ground water divide between the plume and the

municipality. This strategy, for scenario 1^{non}, developed via repetitive simulation runs of MODFLOW, required total industrial pumping of 474,296 ft³/d. Resulting flow from river to aquifer totaled 139,332 ft³/d for the 30 river cells immediately downstream of (10,6). Achieved head differences in layer 1 are at least 0.2 for 5 cell pairs and 0.15 for 3 cell pairs.

TABLE 1. Scenario results.

Scenario	Lower Bound on Total Industrial Pumping	Upper Bound on Flow from River to Aquifer	Total Industrial Pumping	Total Municipal Pumping	Total Flow from River to Aquifer
1 ^{non}			474,296	315,350	139,332
1	267,380*		267,380	315,350	75,123
2			249,086	315,350	68,740
3		139,332*	369,100	416,460	139,332

Units are ft³/day. Extraction is shown as positive for convenience, although it is a negative value in US/REMAX

* Tight bound or constraint. For Scenario 2, a head difference constraint is tight.

The optimization problem objective is to minimize total industrial pumping subject to achieving (at least) the head differences that will keep the plume from moving towards municipal wells.

Optimization results are summarized in Table 1. The optimal strategy computed for Scenario 1 is much less than that developed without optimization (Scenario 1^{non}). It will prevent migration toward the municipal wells. The lower bound on the sum of industrial pumping is a tight constraint. Tight constraints are those which are satisfied exactly, and prevent the objective function value from improving further. None of the head-difference constraints is tight. They are 'loose'. In other words, there is more than 0.2 or 0.15 ft (depending on the pair) difference between the heads at the control locations.

It is appropriate to verify that the computed strategy accomplishes its goal of plume capture, despite application of the linear US/REMAX model to a nonlinear unconfined aquifer. This is done by using the optimal strategy as input to MODFLOW, simulating aquifer response and checking the resulting gradients. Because the system is unconfined there is a very slight error (about 0.01 percent). The error is eliminated by cycling once.

Scenario 2 differs from Scenario 1 in that it does not use a lower bound on total industrial pumping. Results in Table 1 show that 7 percent less than Scenario 1 pumping is actually needed to prevent the plume from moving toward the municipality. The 0.2 head difference constraint between cells (16,18) and (17,18) becomes tight. That constraint prevents pumping from being even lower.

Scenario 3 illustrates how the conflicting objectives involving river dewatering, municipal pumping and plume control can be considered. Assume the consultant wants a strategy that will: (1) maximize total municipal pumping while minimizing total industrial pumping required to satisfy the gradient constraints, (2) have at least as much pumping from each individual municipal well as occurred in Scenario 1^{non}, and (3) not cause the river to lose more water to the aquifer than Scenario 1^{non}.

Table 1 shows the results. The river-aquifer interflow constraint becomes the tight restriction. The model directly computes municipal and industrial pumping rates that achieve the gradient constraints and avoid excessive river dewatering.

The strategy for Scenario 3 actually represents one of a set of optimal strategies for what can be considered a multiobjective optimization problem. It is multiobjective because maximizing municipal pumping and minimizing industrial pumping are two distinct and conflicting objectives. They conflict because as municipal pumping increases, industrial pumping must also increase to keep the control gradients pointed away from the municipal wells.

Alternative pareto optimal strategies belonging to the set of optimal strategies are shown in the curve of Figure 2. Each point on the curve represents one optimal strategy that satisfies the gradient constraints. Here these are developed using the E-constraint method. (The lower bound on total pumping from industrial wells is relaxed in these other optimizations.) Here, the objective function is: maximize municipal pumping. The constraints include bounds on hydraulic gradient and a bound on the sum of industrial pumping. (A lower bound is used because pumping extraction is negative, thus this functions as an upper bound on the absolute value of industrial pumping.) This curve helps involved parties understand the tradeoffs between municipal pumping, industrial pumping, and river-aquifer interflow. A compromise strategy acceptable for all users can be selected.

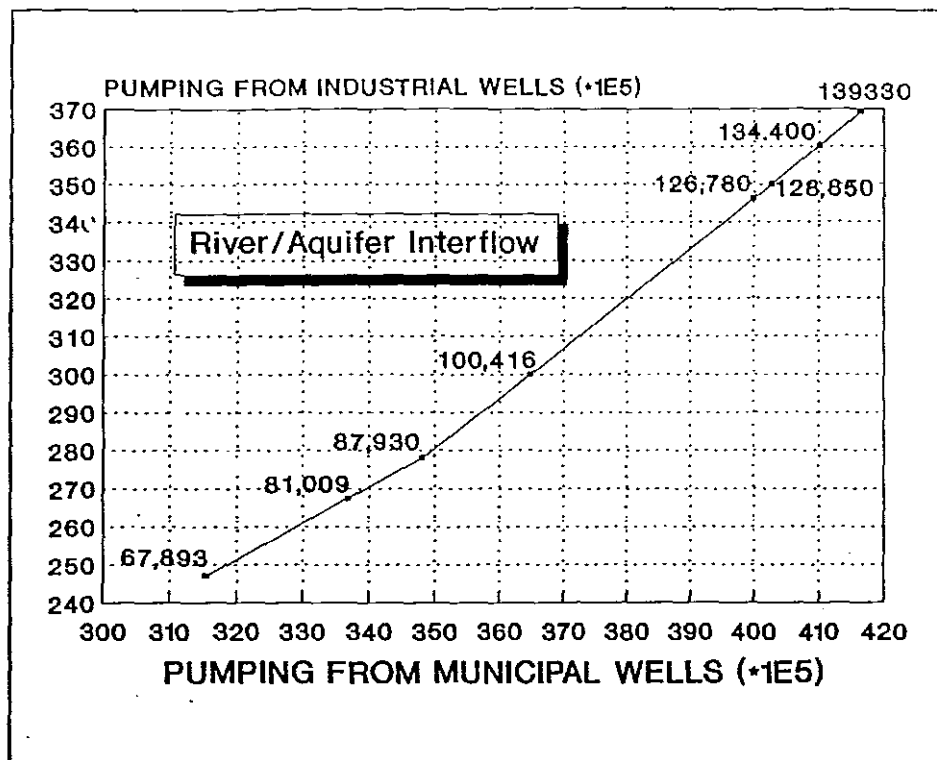


FIGURE 2. Relation between total pumping from municipal wells and total pumping from industrial wells.

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