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.

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WATER IN THE 21ST CENTURY: CONSERVATION, DEMAND, AND SUPPLY
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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. Aly*[1]

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, astrategy 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 variables[2]
    - 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

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[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 Peralt, 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 ft^3/d. Municipal pumping causes the contaminated water to flow toward the northeast, unless the industrial wells pump significantly.

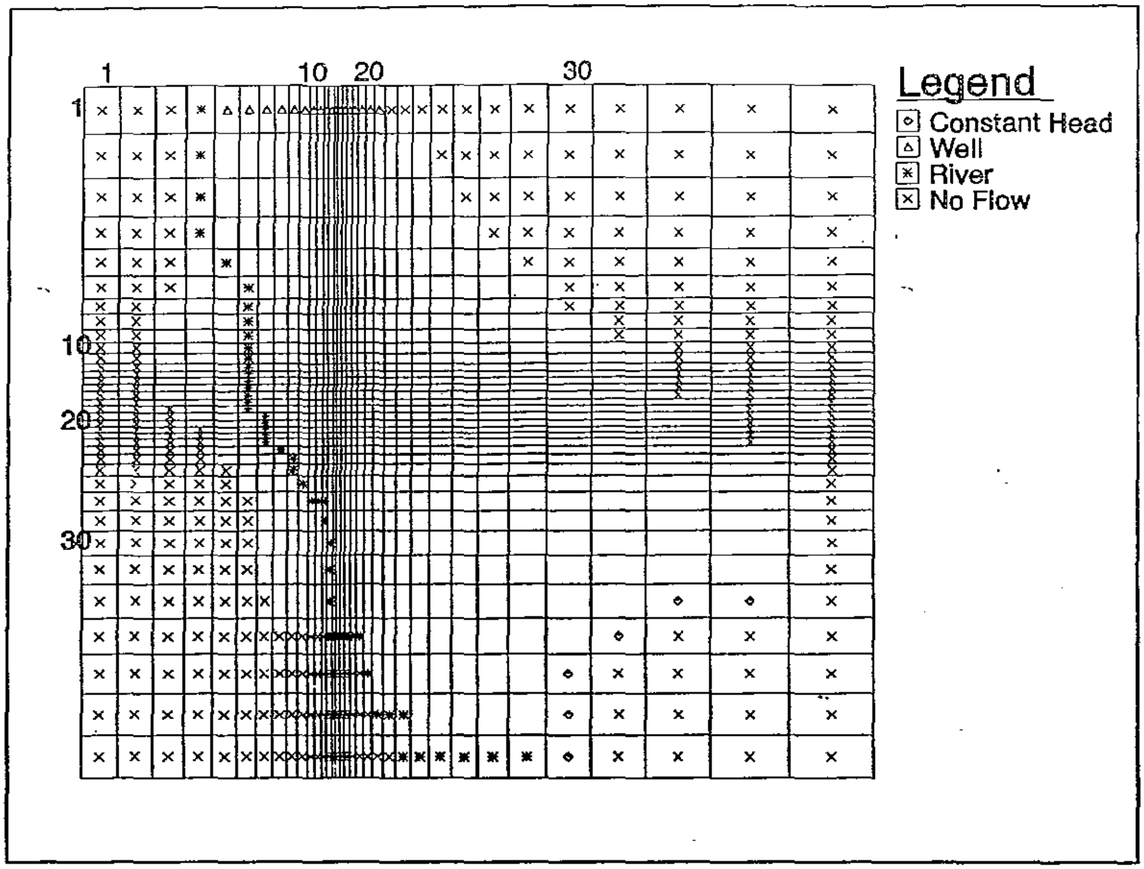

FIGURE 1. Study area; grid and boundary conditions.

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 ft^3/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 ft^3/d. Resulting flow from river to aquifer totaled 139,332 ft^3/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 ft^3/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.

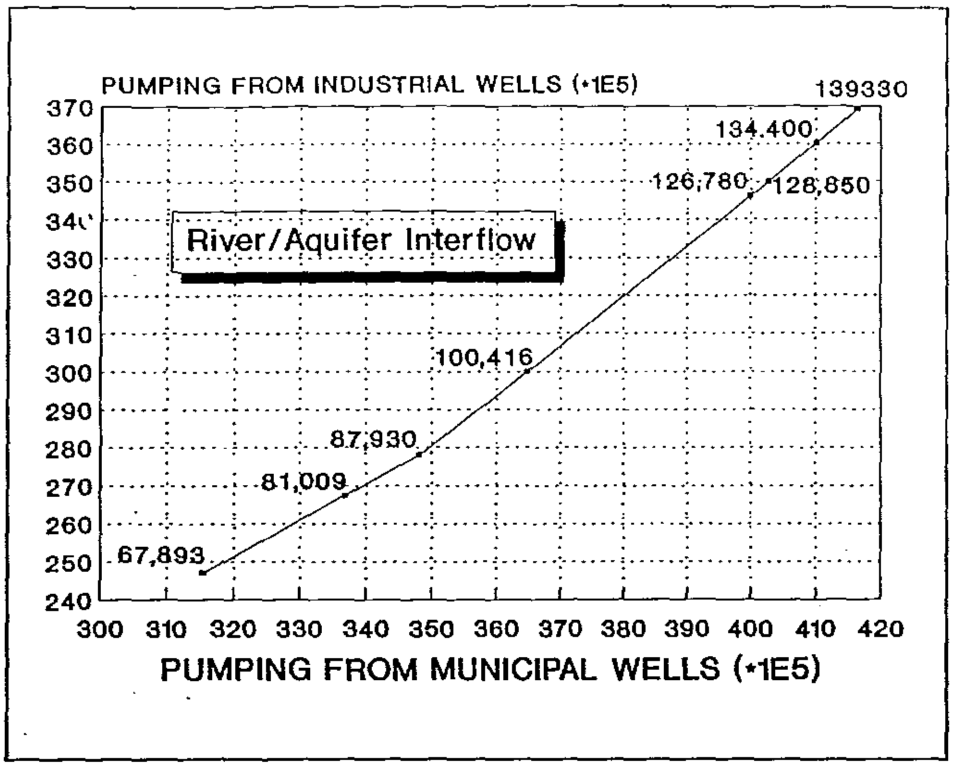

FIGURE 2. Relation between total pumping from municipal wells and total pumping from industrial wells.

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