REMAX: Software for Optimizing Ground-Water Management, Conjunctive Water Management, and Remediation Design

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ABSTRACT

REMAX is a software package designed to assist water managers in developing optimal ground water or coordinated ground water/surface water strategies for a wide range of management problems. REMAX uses MODFLOW, MT3D, and other simulation models to develop the response matrix or response surface equations employed in the final optimization model. To address nonlinear systems (e.g., unconfined aquifers) accurately, REMAX uses a modified response-matrix method. REMAX several nonlinear functions to represent a wide variety of nonlinear response surfaces. REMAX can be used for deterministic or reliability-based optimization problems. Decision variables are ground-water extraction/injection rates and/or surface water diversion rates. State variables include water flows, stages and concentrations. Available objective functions and constraints are linear, nonlinear, integer or mixed integer. REMAX has over 80 objective types including linear, quadratic, integer, goal programming, minimax, and maximin functions. Combining these types for multi-objective optimization makes REMAX ideal for cost minimization and/or utility maximization. Available constraints can be used to define relations among decision variables, state variables, or any combination of these variables in time and space. REMAX has been used for designing several ground-water remediation systems for capture and cleanup of ground-water contaminant plumes.

INTRODUCTION

Competition for water and water quality concerns are intensifying. Needed is improved design and management of groundwater and coordinated ground water and surface water. The ability to predict the effects of management on flow and transport is important. Also critical is the ability to develop optimal management strategies for increasingly complex problems.

Well-documented, verified, and accepted computer models for simulating flow or transport in ground water and surface water resources are used extensively. These simulation (S) models can help guide management decisions. To develop a water management strategy (combination of pumping and/or diversion rates and locations) for a particular situation (scenario), a modeler usually assumes several management strategies. He uses an S model to predict the consequences of implementing each of these strategies. He selects the most desirable strategy from among those assumed. Since there is generally an infinite number of strategies possible for a situation, the chance is slight that the modeler has assumed the absolutely best strategy.

By contrast, a Simulation/Optimization (S/O) model can compute the best management strategy directly (Lefkoff and Gorelick, 1987; Peralta et al., 1989; GeoTrans, 1990; Peralta and Aly, 1993). The modeler defines the management goal(s), and restrictions on acceptable physical system responses. The S/O model calculates the best management strategy for the posed scenario. Here we discuss the most powerful ground water S/O model (REMAX, version 3.00) we know. (Fully-tested version 2.70 for DOS has most of these features and is commercially available).

REMAX FEATURES

Background and Processing Procedure Overview

REMAX assists water managers in developing and selecting optimal ground-water pumping (extraction and injection) and conjunctive water management strategies for a wide range of management problems. REMAX computes optimal pumping and diversion rates and resulting physical system responses using Response Matrix (RM; adapted for nonlinear systems) and Response Surface (RS) methods. REMAX combines ground-water flow and transport simulation, open channel flow simulation, and operations research optimization capabilities.

To simulate system responses (aquifer head, contaminant concentrations, contaminant mass, drain-, river-, or stream-aquifer interflow, stream stage, and stream outflow) to pumping and/or diversion, REMAX uses either superposition expressions (RM) or neural networks (RS Method).

REMAX requires input data concerning the physical system and stresses not subject to optimization. These include the same data needed to run the normal simulation (S) models MODFLOW (Harbaugh and McDonald, 1996) , MT3D (Zheng, 1990), or SWIFT (Reeves et al, 1986). REMAX also requires data defining management goals for formulating the management problem.

After reading physical system data, REMAX initially computes the nonoptimal head changes resulting from existing stresses (a non-optimal scenario). Then if the user selects the RM method, REMAX calculates influence coefficients describing system response to unit hydraulic stimuli (ground-water pumping or surface-water diversion). If the user selects the RS method, REMAX carries out numerous system simulations and uses these simulations to develop response-surface expressions or to train and test the artificial neural networks. Then, REMAX organizes the user-specified optimization problem (including objective function, locations of decision stimuli, locations at which state variables are to be constrained, and all other constraints and bounds). An optimization algorithm then calculates an optimal water use strategy for the posed management problem.

The optimization problem solved for the manager includes an objective function (OF), constraints and bounds. The OF and constraints are equations consisting of coefficients and variables. The model will determine the set of values of the variables that maximize or minimize the OF value, while satisfying all constraint and bound equations. All computed variable values will lie within the upper and lower bounds set by the user.

Objective Functions

REMAX has over 80 hard-coded OF types to choose from. Included are linear, quadratic, nonlinear, integer, and nonsmooth. Any of these OF types can be combined for multiobjective optimization using weighting or E-constraint methods. OF options include:

- Linear objective. OF value is a linear combination of decision variables (pumping and/or diversion rates) and/or state variables (heads, flows, concentrations, contaminant mass).
- Quadratic objective. OF value includes products of decision and state variables (for example pumping rates times pumping lift or total dynamic head).
- Binary or mixed integer objective. Integer variables can be used to represent number of pumping wells or diversion points. If an integer variable is multiplied by the cost of installing a well, a mixed integer OF can be used to minimize the pumping system installation cost.
- Goal programming with absolute penalty objectives. OF value is the sum of absolute-valued deviations from prespecified goals. Any decision or state variable can be a goal. Assigning different penalty coefficients to upward or downward deviations allows emphasizing over- or under-achievement of goals. This type of OF can be used to determine how to most closely achieve any specified goals that might not be perfectly attainable.
- Goal programming with quadratic penalty objectives. OF value is the sum of squared deviations from prescribed goals. Any decision or state variable can be a goal.
- Goal programming with maximum penalty objectives. OF value is the maximum deviation of a variable from its prescribed goal. Any decision or state variable can be a goal.
- Maximin and Minimax objectives. These objectives minimize the maximum value (or maximize the minimum value) of a given specified decision or state variable resulting from optimization.

For flexibility, the user can assign weights to variables included within OFs. In this way, for example, one can either minimize or maximize ground water pumped. For regional planning, one might want to maximize sustainable ground-water extraction. For ground-water contaminant plume remediation, one might want to minimize the pumping needed to contain the plume or minimize the residual contaminant mass at the end of the planning horizon. Weighting coefficients permit emphasizing pumping from individual (or groups of) pumping or diversion locations. Weighting coefficients (weights) can represent unit costs for economic optimization.

Constraints

REMAX includes five general categories of constraint equation types:

1. Constraints describing effect of decision variables on state variables. If the Response Matrix Method is used, these constraints are linear superposition equations. For the Response Surface Method, these constraints are implemented as linear or nonlinear functions or artificial neural networks. Constraints define responses of aquifer head, drain-, river- or stream-aquifer interflow, stream stage, outflow from a stream reach, contaminant concentration, mass of contaminant removed, residual contaminant mass, and other nonlinear variables (Ejaz and Peralta 1995a,b; Cooper et al. 1998).

2. Constraints specifying restrictions for groups of decision or state variables. Users can specify groups of pumping wells, stream diversions, or both combined. Users can specify lower and upper bounds on total flow for each group. Integer programming capabilities permit setting upper limits on the number of active members in each group. Users can optionally control total drain-, river-, or stream-aquifer interflow in groups of cells or combinations of groups.

3. Constraints describing temporal relationships between decision variables. Users can employ temporal monotonicity constraints for pumping and/or diversion rates. Montonicity constraints are sometimes used for regional planning if legally permitted pumping rates should not decrease from one year to the next year.

4. Constraints describing relations between pairs of variables. These are used to constrain ground-water gradients (or velocities). Gradients are functions of head differences. Users can pair any two head control cells to form a gradient variable. The paired head control cells need not be in the same layer, permitting both vertical and horizontal control.

5. Simple bounds constraints. Users can specify lower and upper bounds on all variables in the optimization models. In E-constraint multiobjective optimization, one bounds the objective value for some of the employed objectives.

Unique or Special Features

1. Well-proven, diverse simulation modules to address porous and fractured media. REMAX is appropriate for optimizing flow and transport management in heterogeneous multilayer porous or fractured aquifers. To develop influence coefficients describing hydraulic head or flow response to stimuli, REMAX uses MODFLOW and MT3D for porous media simulation or SWIFT for fractured media. Other simulation models are easily added as necessary.

2. Robust and proven optimization solvers. REMAX contains all software needed to solve the described optimization problems.

3. Easily maintained data sets. For any particular problem, REMAX reads all data files from a user-specified subdirectory (or folder in WIN95/NT). This allows REMAX users to save all problem-specific input and output in a distinct location.

4. User-friendly data files, error checking, and diagnostics. Innovative REMAX input file organization allows users to write comments, use blank lines, or use blank spaces as desired. This permits thorough data set documentation. REMAX also checks every input file entry and generates error messages with diagnostic explanations.

5. Compatibility with other software. REMAX can standard MODFLOW, MT3D and SWIFT data sets. Users can prepare these files using their preferred pre-processor and use the generated input files within REMAX.

6. Ability to compute head at well casing or at cell center. This feature is useful for managing unconfined aquifers of small saturated thickness and for computing hydraulic lift costs.

7. Ability to address systems in which pumping cells or head control cells might initially be or might become fully dewatered. This nonlinear or piecewise linear problem is not addressed by normal response matrix models.

8. Automatic cycling and post-optimization simulation. This enables users to accurately address nonlinear systems (unconfined aquifers and stream/aquifer systems). Cycling proceeds until user-specified maximum number of cycles or convergence criteria for decision variables are achieved. Post-optimization simulation verifies that the results in the nonlinear physical system should be like those in the optimization model.

9. Almost infinite flexibility in addressable problem types. Any of the different types of objective functions can be combined into composite objective functions. Any type of the mentioned constraints can be used with any of the objective function types.

10. Optimization under uncertainty or for risk management. Optimization can satisfy constraints for an unrestricted number of sets of assumed boundary conditions and aquifer parameters (realizations) simultaneously. Reliability of computed strategies is determined via Monte Carlo post optimization simulation. This feature can be used with any combination of objective function(s) and constraints.

11. Ability to develop cost-reliability tradeoff curves (Aly and Peralta, 1998). This ability is provided by the following features:
    - optional use of head at well casing instead of average cell heads.
    - use of quadratic objective function including pumping rate, volume, and cost.
    - use of binary and mixed integer variables to include cost of well installation or water treatment plant sizing within the optimization.
    - coupled use of cost optimization with the multiple realization option.

12. Adaptability for special situations (available within a special version). Additional constraints can be added as needed, such as those for: (1) managing reservoir releases and conjunctive water delivery to a system of irrigation unit command areas (Belaineh et al, 1998); or (2) assuring that legal water right priorities are satisfied (Assume two adjacent surface water users. User 1 has a higher legal water right than User 2. Special constraints can assure that User 2 will not receive any water unless all of User 1 water right is satisfied).

Assumptions and Adaptation for Nonlinear Systems

For extremely nonlinear systems, the user might prefer to employ REMAX's Response Surface methods (nonlinear equations or artificial neural networks; ANNs). ANNs are used to simulate all state variables within the optimization algorithm. ANNs are very powerful universal approximation tools. They can simulate the most complex nonlinear behaviors.

If the user chooses the Response Matrix method to describe ground-water hydraulics, REMAX utilizes linear systems theory and superposition. 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. To appropriately address the nonlinearity, MODFLOW treats that as a linear process during a single iteration, but changes transmissivity with each iterative solution of the flow equation. Processes represented as piecewise linear in MODFLOW include drain-, river-, and stream-aquifer interflow, evapotranspiration, and vertical flow between layers.

REMAX adapts to significantly nonlinear system response via cycling. A common rule of thumb is to assume that horizontal ground-water 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 that error to much less than 5 percent in REMAX by cycling (Peralta and Kowalski, 1988; Takahashi and Peralta, 1995). 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.

In summary, REMAX applies perfectly to linear systems. When addressing nonlinear systems (e.g. unconfined aquifers), accuracy is enhanced by using either the Response Surface method or cycling. Determining whether/how much to cycle involves considering how well the simulation model is calibrated and how well the aquifer is characterized.

SUMMARY

REMAX can aid developing optimal water management strategies for aquifer and stream-aquifer systems. It performs linear, quadratic, nonlinear or mixed integer optimization. It contains a very large number of hard-coded objective function types to perform deterministic or stochastic optimization or multi-objective optimization. REMAX includes linear, integer, and nonlinear constraints. REMAX uses either an automated cyclical superposition approach or artificial neural networks to describe aquifer heads, contaminant mass and concentration, drain-, river-, and stream-aquifer interflow, stream stage, and streamflow to ground-water pumping and surface water inflows or diversions. REMAX also uses a wide range of linear and nonlinear constraint equations to describe contaminant concentrations (in surface water and ground water), light-non-aqueous phase liquid (LNAPL) head, or LNAPL volume (free product, residual, or extracted) response to water management. Using such constraints, REMAX can be used to optimize attainment of target contaminant concentrations, aqueous or non aqueous phase contaminant removal or capture and general ground water and conjunctive water management. REMAX permits binary and mixed integer constraints. In economic optimization this permits controlling the number of wells that can be active in a given time period. Users can control flows from specified groups of wells and/or stream diversions. REMAX contains all needed simulation and optimization algorithms.

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