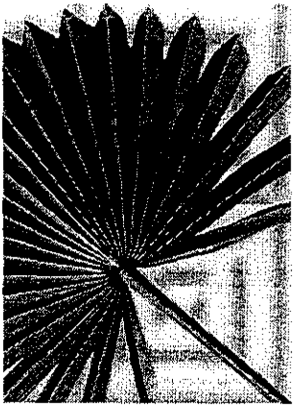
Sixth International Conference on Computers in Agriculture



Cancun, Mexico
June 1996

Published by
American Society of Agricultural Engineers

Editor
Fedro S. Zazueta

Co-Editors
Polioptro Martínez-Austria
Jiannong Xin
Nahún H. García-Villanueva

Software for Optimizing Groundwater or Conjunctive Water Management

Richard C. Peralta and Alaa H. Aly[1]

Abstract

US/REMAX is a computer program designed to assist water managers in developing optimal groundwater and/or surface water strategies for a wide range of management problems. It employs response matrix, regression and other methods adapted for nonlinear systems. US/REMAX performs deterministic or reliability-based, single- or multi-objective optimization. Decision variables are ground-water extraction/injection and/or surface water diversion. State variables include water flows, stages and concentrations. Hard coded objective functions and constraints are linear, nonlinear, integer or mixed integer. Special constraints can be added to address unusual situations.

KEY WORDS: simulation/optimization model, conjunctive water management, groundwater, contamination, optimization.

Introduction

As competition for water and concern about water quality intensify, managers should improve coordinated management of ground water and surface waters. The ability to predict the effects of management practices on surface and groundwater flow and contaminant 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 groundwater and surface water resources exist. 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 the 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.

On the other hand, a Simulation/Optimization (S/O) model can compute the best management strategy directly (Lefkoff and Gorelick, 1987; 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 management scenario. Here we discuss capabilities of the most powerful groundwater S/O model (US/REMAX, version 2.70) we are aware of.

US/REMAX Features

Background and Processing Procedure Overview

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 Response Matrix (adapted for nonlinear systems) and regression methods. US/REMAX combines groundwater and open channel flow simulation with operations research optimization capabilities.

---

[1] Richard C. Peralta, Professor, Biological and Irrigation Engineering, Utah State University, USU/DBIE, Bldg EC-216, Logan, Utah 84322-4105, USA, email peraltar@lab.cee.usu.edu (801) 797-2786; Alaa H. Aly, Ph.D. candidate, email slmdh@cc.usu.edu.

To simulate system responses (aquifer head, drain-, river-, or stream-aquifer interflow, stream stage, and steam outflow) to pumping and/or diversion, US/REMAX uses superposition expressions. It uses other linear and nonlinear equation types to describe response of contaminant concentration, mass of contaminant removed, residual contaminant mass, and other variables.

US/REMAX requires input data concerning the physical system and stresses not subject to optimization. These include much of the same data needed to run the normal simulation (S) models MODFLOW (McDonald and Harbaugh, 1988) , STR (Prudic, 1989), or SWIFT (Reeves et al, 1986). In addition, US/REMAX requires data concerning management goals for formulating the management problem.

After reading physical system data, US/REMAX initially computes the nonoptimal head changes resulting from existing stresses (a non-optimal scenario). Then it calculates influence coefficients describing system response to unit hydraulic stimuli (groundwater pumping or surface-water diversion). The model organizes the user-specified optimization problem which includes objective function, locations of optimizable 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 that is solved for the manager consists of an objective function, constraints and bounds. The objective function 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 value of the objective function, 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

US/REMAX has over 80 hard-coded objective function types for the user to choose from. Included are linear, quadratic, nonlinear, integer, and nonsmooth objective functions. Any number of these functions can be combined for multiobjective optimization using weighting or E-constraint methods. Objective function options include:

- Linear objective. Objective function value is a linear combination of decision variables (pumping and/or diversion rates) and/or state variables (heads, flows, concentrations).
- Quadratic objective. Objective 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. When the integer variables are multiplied by the cost of installing one well, a mixed integer objective function can be used to minimize the cost of installed pumping system.
- Goal programming with absolute penalty objectives. Objective value is the sum of absolute-valued deviations from prespecified goals. This objective function is available for all decision and state variables used within US/REMAX. Different penalty coefficients can be assigned by users to upward and downward deviations to allow emphasizing over- and under-achievement of goals. This type of objective function 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. Objective value is the sum of squared deviations from prescribed goals. This objective function is available for all decision and state variables within US/REMAX.
- Goal programming with maximum penalty objectives. Objective value is the maximum deviation of a variable from any prescribed goal. This objective function is available for all decision and state variables within US/REMAX.
- Maximin and Minimax objectives. These objectives minimize the maximum value (or maximize the minimum value) of a given type of decision or state variable that results from optimization.

For flexibility, the user can assign weights to variables included within appropriate objective functions. In this way, for example, one can either minimize or maximize groundwater pumped. In a regional planning scenario one might want to maximize sustainable groundwater extraction. In a groundwater contaminant plume remediation effort one might want to minimize the pumping needed to capture the plume. Weighting coefficients can be used to emphasize pumping from individual (or groups of) pumping or diversion locations. Weighting coefficients (weights) can represent unit costs for economic optimization.

Constraints

US/REMAX includes five general categories of constraint equation types:

1. Constraint equations to describe effect of decision variables on state variables. These constraints can either be linear superposition equations, or other linear or nonlinear equations. Constraint equations define response 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.

2. Constraint equations to specify restrictions for groups of decision or state variables. Users can specify any number of groups of pumping wells, stream diversions, or both combined. Users can specify lower and upper bounds on the total flow rate for each group. Integer programming capabilities allow users to set 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. Constraint equations to describe temporal relationships between decision variables. Users can optionally 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. Constraint equations to describe relations between pairs of variables. These equations are used to constrain groundwater 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 a variable representing the value of one of the objectives can be bounded.

Unique or Special Features

1. Well-proven, diverse simulation modules to address porous and fractured media. US/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, US/REMAX uses MODFLOW, MODFLOW with STR, or SWIFT-- widely used S models. Other S models are easily added as necessary. A US/REMAX utility program uses MT3D to help create nonlinear relationships between pumping and contaminant concentrations (and other state variables). These surrogate equations are used as constraints within US/REMAX. MODFLOW and MT3D address porous media. SWIFT addresses fractured media.

2. Easily maintained data sets. For any particular problem, US/REMAX reads all data files from a user-specified subdirectory. This allows US/REMAX users to save all problem-specific input and output in a distinct directory.

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

4. Ability to read normal MODFLOW, STR and SWIFT data sets. One doesn't need to modify such data sets for use with US/REMAX. However, specified output control options must be used to cause appropriate S model output.

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

6. 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.

7. 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.

8. Almost infinite flexibility in type of problem addressed. 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.

9. 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.

10. Ability to develop cost-reliability tradeoff curves. 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.

11. Adaptability for special situations (available for a special version). Additional constraints can be added as needed, such as those for managing reservoir releases and conjunctive water delivery to a system of irrigation unit command areas (Belaineh et al, 1995). A more recent example includes piecewise linear constraints (or nonlinear surrogates) such as those needed to assure that legal water right priorities are satisfied during optimization. For example, assume two adjacent surface water diverters. User 1 has a higher legal water right than User 2. Special constraints can be added to assure that User 2 will not receive any water unless all of User 1 water right is satisfied.

Assumptions and Adaptation for Nonlinear Systems

To describe groundwater hydraulics, US/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.

US/REMAX adapts to significantly nonlinear system response via cycling. 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 that error to much less than 5 percent in US/REMAX 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.

Concentration response to an initially unknown pumping strategy can be nonlinear. US/REMAX includes linear and nonlinear expressions to describe aqueous or NAPL contaminant response to pumping. Forms include those used by Ejaz and Peralta (1995), Cooper, et al. (1995), Peralta and Aly (1995), and others.

In conclusion, 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.

Summary

The US/REMAX software package can aid developing optimal water management strategies for aquifer and stream-aquifer systems. It performs linear, quadratic, nonlinear or mixed integer optimization. It permits the user to select from a very large number of hard-coded objective function types to perform deterministic or stochastic optimization or multi-objective optimization. US/REMAX includes linear, integer, and nonlinear constraints. US/REMAX uses an automated cyclical superposition approach to describe aquifer heads, drain-, river-, and stream-aquifer interflow, stream stage, and streamflow to groundwater pumping and surface water inflows or diversions. US/REMAX also uses a wide range of linear and nonlinear constraint equations to describe contaminant concentrations (in surface water and groundwater), light-non-aqueous phase liquid (LNAPL) head, or LNAPL volume (free product, residual, or extracted) response to water management. Using such constraints, US/REMAX can be used to optimize attainment of target contaminant concentrations, aqueous or non aqueous phase contaminant removal or capture and general groundwater and conjunctive water management. US/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.

References

Belaineh, G., Peralta R., and Hughes, T. 1995. *Enhanced simulation/optimization modelling for conjunctive management of reservoir/stream/aquifer systems.* System Simulation/Optimization Laboratory Report 95-1, Dept. of Biological and Irrigation Eng., Utah State University, Logan, Utah. 45 p.

Cooper, G., Peralta, R. C., and J. J. Kaluarachchi. 1995. *Optimizing separate phase light hydrocarbon recovery from contaminated unconfined aquifers.* System Simulation/Optimization Laboratory Report 95-2, Dept. of Biological and Irrigation Eng., Utah State University, Logan, Utah. 48 p.

GeoTrans, Inc. 1990. Documentation and user's guide for MODMAN: An optimization module for MODFLOW, Version 2.0. GeoTrans, Inc. Herndon, Virginia. 358 p.

Gharbi, A. and Peralta, R.C. 1994. "Integrated embedding optimization applied to Salt Lake Valley aquifers," Water Resources Research, 30(4), pp. 817-832.

Ejaz, M. S. and R. C. Peralta. 1995. "Maximizing conjunctive use of surface and groundwater under surface water quality constraints." Advances in Water Resources. 18(2):67-75.

Lefkoff, L.J. and Gorelick, S.M. 1987. AQMAN: linear and quadratic programming matrix generator using two-dimensional ground-water flow simulations for aquifer management modeling. Water Resources Investigations Report 98-4061, USGS, Menlo Park, California.

McDonald, M. G. and Harbaugh, A. W. 1988. A three-dimensional finite-difference groundwater model, U.S. Geological Survey, Open File Report 83-875.

Peralta, R.C. and Aly, A. 1993. US/REMAX (Utah State Model for Optimizing Management of Stream/Aquifer Systems Using the Response Matrix Method) User's Manual. Software Engineering Division, Biological and Irrigation Engineering Dept., Utah State Univ., Logan, Utah. 200 p.

Peralta, R. C. and Aly, A. 1995. *Optimal Pumping Strategies to Maximize Contaminant Extraction of TCE Plume at Central Base Area, Norton AFB, California,* Water Studies Report Number II, Air Force Center for Environmental Excellence, Environmental Restoration Directorate. 29p.

Peralta, R.C. and Kowalski, K.G. 1988. "Optimal volumetric and economic groundwater mining for the Arkansas Grand Prairie," Agricultural Water Management, 15, pp. 1-17.

Prudic, D.E. 1989. "Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model". U. S. Geological Survey. Open-file Report 88-729. Government Printing Office, Washington, D.C.

Reeves, M., Ward, D.S., Johns, N.D., Cranwell, R.M. 1986. Theory and Implementation for SWIFT II, the Sandia Waste-Isolation Flow and Transport Model for Fractured Media, Release 4.84, NUREG/GR-3328, SAND83-1159, Sandia National Laboratories, New Mexico, 189 p.

Reilly, T. E., Franke, O. L. and Bennett, G. D. 1987. "The principle of superposition and its application in ground-water hydraulics". Techniques of Water-Resources Investigations of the U. S. Geological Survey, Book 3, Chapter B6. Department of the Interior. U. S. Geological Survey.