SOMOS
Simulation/Optimization Modeling System

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ABSTRACT

SOMOS (Simulation / Optimization Modeling System) is a family of simulation / optimization (S/O) modules to aid in optimally managing water resources. SOMOS results from twenty years experience developing optimization models and applying them to real-world problems, including 11 pump-and-treat (PAT) systems and numerous water supply problems. SOMOS significantly improves water management or designs and saves money. Its user's manual provides excellent training in principles of applying optimization to managing aquifer and stream-aquifer systems. It is being incorporated with powerful groundwater modeling and visualization packages.

INTRODUCTION

How does one know where to place well screens and how much to extract or inject in order to least expensively control or remediate ground-water contamination? How does one know where and how much fresh water to inject to prevent salt-water intrusion, or to manage artificial recharge and eventual recovery? How does one know how best to coordinate use of groundwater and surface water resources for water supply? For these purposes, SOMOS is the most powerful, and flexible software my research group is aware of (SSOL, 2002). SOMOS can help inexperienced and experienced modelers develop optimal water management strategies.

A pumping (or management) 'strategy' is a set of spatially and perhaps temporally distributed water or chemical injection/extraction rates—in other words, where and how much to inject or extract to/from the aquifer. A strategy can consist of the flow rates to be extracted at cells of a modeled aquifer. A 'design' can contain the rates and locations, and specifications of hardware systems. 'Optimal' strategies and designs are the best that can be developed for the posed optimization problems. Optimization problems are usually described using an objective function, constraints and bounds. An optimal strategy developed for a specified 'scenario' is optimal for that scenario, but is often sub-optimal for a different one. An optimization problem scenario is sometimes referred to as a 'formulation'. A scenario/formulation includes all assumptions needed to specify the optimization problem and to apply the appropriate simulation model. Sometimes scenario/formulation also refers to the strategy developed for a scenario/formulation.

Modelers must input management strategies into Simulation (S) models such as MODFLOW and MT3DMS. S models predict how a physical system will respond to an input strategy. S/O models differ in that they will produce an optimal management strategy for an assumed management problem. That means that the user must input data to describe the management problem. S/O models are better than S models for developing management plans. S/O models must include a way of predicting system response to management. S/O models include S models or substitutes.

Table 1 illustrates differences between S and S/O model inputs and outputs. Note that the S/O model user must input the locations of an individual or a region of candidate wells. A candidate well is one that the user wants the S/O model to consider in its optimization. The model will decide whether or not the well should be used, and at what rate it should pump. If the user wishes SOMOS to consider a large number of well locations, SOMOS can easily do so, while selecting only the best location for the optimal management strategy that it recommends. Sometimes, the longer an individual computer simulation takes to run, the fewer simulations one wants the S/O model to make—i.e. the fewer unnecessary candidate wells one wants the S/O model to consider. SOMOS makes it easy for an experienced hydrologist or S model user to capitalize on his expertise. Groundwater experience is enhanced by using SOMOS. This is especially true as it is merged with graphically-based pre- and post-processors.

Model Type	Input Values	Computed Values
Simulation (S)	Physical system parameters	
	Initial & boundary conditions	Some heads, flows, concentrations
	Extraction & recharge rates	
Simulation/ Optimization (S/O)	Physical system parameters	
	Initial and boundary conditions	Some optimal boundary conditions
	Candidate decision variable locations. Bounds on flux rates, heads, flows, concentrations. Other restrictions.	Optimal pumping, heads, flows, concentrations
	Objective function (equation)	Objective function value

Table 1. Partial Comparison between Inputs and Outputs of Simulation (S) and Simulation/Optimization (S/O) Models

REAL-WORLD APPLICATIONS

Table 2 shows PAT situations in which our team has applied S/O models to a site assuming the same initial and boundary conditions as an experienced consultant applied trial-and-error design using only S models. Peralta et al. (2003) discuss the projects. Peralta (2001a) discusses some of our other S/O model-developed PAT strategies. Table 2 demonstrates a range in benefits that one can expect from S/O model use. A twenty percent improvement in strategy is a reasonable expectation for problems in which there is freedom for the optimization to perform. This was achieved for sites at Umatilla (Oregon), Blaine (Nebraska) and Norton (California). Results for Oregon, Utah, and Nebraska were for the Environmental Security Testing and Certification Program (ESTCP).

Our Blaine PAT strategy is a highly regarded accomplishment, partially because of problem complexity (60 stress periods, long plume, multiple contaminants), (SSOL, 2002b). Umatilla and Norton were much simpler problems. Our Umatilla strategy shines because it is robust compared with hundreds of other designs of equally low cost (SSOL, 2002d). Our Norton design represents successful innovative injection use. Given freedom for optimization SOMOS performs magnificently.

Our MMR strategy is compared to a preliminary final design prepared by a consultant. S/O model benefit was not great because the problem was tightly constrained—including the need to avoid spreading contamination through formerly clean aquifer. That design has yielded excellent mass removal in the field. The identified Tooele plume containment problem could be addressed with several extraction wells—as the S model user and we did. Both extracted the entire plume (>5ppb) that was nearing the boundary of the containment zone. Less costly would be to inject water to push the plume away from the boundary. We did not take that approach because it would force contamination above MCL (>5ppb) into relatively clean aquifer (<5ppb), causing spreading and reducing mass removal compared with an extraction approach (Peralta et al., 2003; SSOL, 2002c).

Site	UMATILLA	TOOELE	BLAINE	MASSACHUSETTS MILITARY RESV. CS-10	NORTON
State	Oregon	Utah	Nebraska	Massachusetts	California
Model size (lay-row-col)	5 - 132 - 125	4 - 165 - 99	6 - 82 - 136	21 - 161 - 159	3 – 77 - 72
Modeling period (yrs)	20	21	30	30	15
Stress periods	4	7	60	5	1
Contaminants	RDX, TNT	TCE	TCE, TNT	TCE	TCE
Formulation 1[(a)] (min cost)	$1.66M	$14.14M	$40.82M	2900 kg	$24.75
Improvement from base strategy [(e)]	20%	3%	19.9%	6% [(f)]	23%
Formulation 2[(b,h)] (min cost)	$1.66M	-	$18.88M	-	-
Improvement from base strategy	20%	-	33.5%	-	-
Formulation 3[(c,h)]	0.20 kg	-	2139 gpm[(g)]	-	-
Improvement from base strategy	47%	-	26%	-	-
Formulation 4[(d)]	$1.66M / 0.2 kg	$16.98M	-	-	-
Improvement from base strategy	20% / 47%	-	-	-	-
Status of Designed System	Paper Study	Paper Study	Paper Study	Constructed. Successful	Constructed. Successful

(a) MMR primary objective was to maximize dissolved TCE extraction. We developed a mass removal - cost trade-off curve.

(b) For Umatilla, Tooele and Hastings, Formulation 2 differs from Formulation 1 in constraints

(c) Formulation 3 is minimize mass remaining, min. cost, and min-max. pumping for Umatilla, Tooele and Hastings, respectively

(d) Formulation 4 combines F1 and F3 for Umatilla. For Tooele, F4 is a min. cost problem using modified Form. 3 constraints. We prepared Formulation 4 designs to satisfy our curiosity. We did this after a first project deadline.

(e)Computed as {(S Design Value) – (SO Design Value)} / (S Design Value)

(f) 6 % more mass removed than 'Run57'. Later, we reduced cost by $0.54M without significantly affecting mass removal.

(g) SOMOS produced a 2123 gpm strategy several days after the first project deadline (SSOL, 2002b)

(h) For Tooele, only our Formulation 1 strategy is directly comparable to a strategy developed using S model trial-and-error. Our strategies should not be contrasted with strategies that inject, forcing contamination into relatively clean aquifer, or inject in hot-spots to reduce concentrations to below MCL by dilution. Peralta et. al (2003) and SSOL (2002c)

Table 2. Selected Comparisons of PAT Strategies USU developed by S/O Model versus Strategies Developed by Experienced Consultants Using S Model Trial-and-Error

SOMOS results from many years of applying optimization to large and small scale groundwater and conjunctive water management issues. It or evolutionary precursors (most recently REMAX, REMAXIM) have been used for a wide range of problems and simulators (MODFLOW, STR, MT3DMS, SWIFT, QUAL2E, ARMOS, SEAWAT, etc.) by students and staff. Examples include developing management strategies for (Peralta, 2001a,b; Peralta et al., 2003): aqueous and non-aqueous plume management; regional sustained groundwater yield; salt water intrusion prevention; dynamic time-varying stream-aquifer-reservoir-drain conjunctive use; surface water waste loading and water quality; multi-objective optimization where environmental and water supply goals conflict. SOMOS' applications increase as new problem types are brought to us.

SOMOS FEATURES

Tailored Module Design Concept

The author's experience with groundwater optimization modeling has included problems wherein over a thousand pumping rates were optimized, and thousands of state variables were constrained (Peralta, 2001b). Some simulation models have been complex with many layers and stress periods. We have developed many techniques for developing optimal solutions for complicated linear and nonlinear optimization problems.

SOMOS is designed to take advantage of the fact that different S/O approaches are best for different groundwater problem types. SOMOS has modules tailored for different problem types. Of course, for simplicity, data input formats, except module-specific needs, are the same for all modules. Modules employ proven numerical flow and/or transport models plus surrogate response surface simulators to predict system response to management. They also include 14 optimization algorithms (many of them world-renowned) enabling the user to employ defaults or hand-select the solver most suitable for different types of optimization problems. This article discusses SOMOS modules SOMO1 and SOMO3.

SOMOS is designed to allow the groundwater professional to best utilize his skills in the man-machine process of developing optimal water management strategies. SOMOS provides many operational features to this end. Figure 1 illustrates some SOMO3 operations.

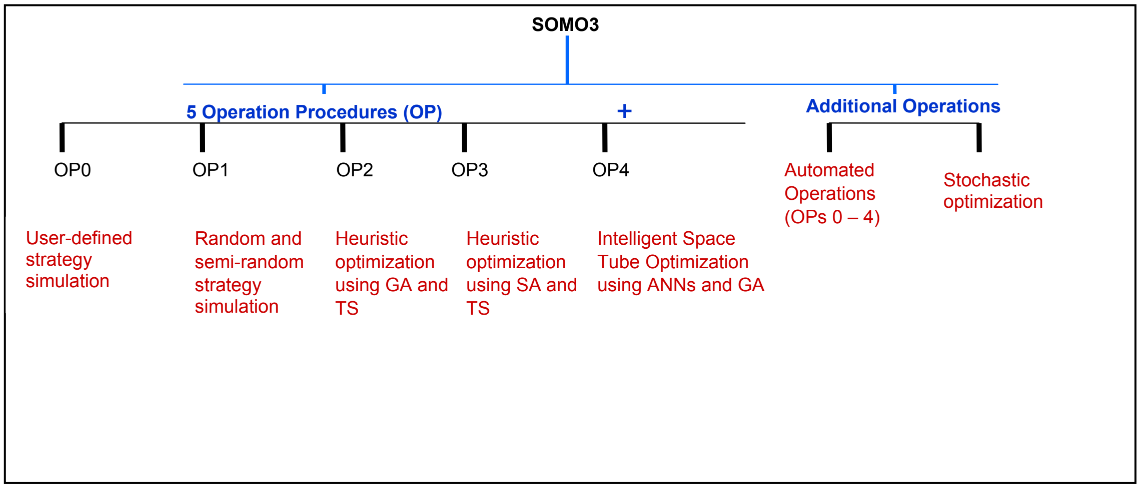

Figure 1. Overview of Major SOMO3 Operations

Simulators

All SOMOS versions come with MODFLOW and MT3DMS. Higher versions have other simulators or can use any simulator that produces text file output. For computational efficiency, module SOMO1 uses response matrix (RM), polynomial and other response functions as substitute simulators. SOMO3 also uses artificial neural networks (ANNs) as surrogates. SOMOS verifies the accuracy of all surrogates so they are confidently used.

Optimization Algorithms and Problem Types

SOMO1 is ideal for any scale of hydraulic optimization problems up to very large sizes having thousands of decision and state variables, depending on the SOMO1 version utilized. If needed, it can include transport optimization with those hydraulic problems. SOMO1 performs optimization using operations research (OR) algorithms (such as simplex, gradient search, branch and bound, and outer approximation). SOMO1 has with it 10+ commercial solvers, including MINOS and DICOPT. With these solvers SOMO1 addresses linear, nonlinear, mixed integer, mixed integer nonlinear, multi-objective and stochastic optimization problems. SOMO1 can be linked to GAMS models to ease large-scale economic modeling.

SOMO3 addresses the same problem types and can use heuristic optimization (HO), including genetic algorithm (GA), simulated annealing (SA), and integrated tabu search (TS). SOMO3 is ideal for complex groundwater contamination management. One pump and treat problem addressed recently included 21 model layers, and a 30 year planning horizon. Another involved simultaneously optimizing 25-well time varying pumping for five 5-year periods.

Objective Functions, Variables, and Constraints

SOMOS:
- Can optimize for 90+ distinct management goals (objective functions) plus user-defined objective
- Can constrain all pertinent variables (pumping, stream diversion, flows, cell head, head just outside well casing, concentration, user-defined)
- Has unique tools, including stochastic optimization, for increasing strategy robustness and reliability under uncertainty
- Performs multi-objective optimization

Other Features

- Windows-based SOMOS runs in computer background, while user employs other programs.
- SOMOS' spread-sheet based pre-processor, SOMOIN, simplifies input file preparation.
- SOMOS has detailed input error-checking and error messages.
- Buttons on SOMOS' user-friendly interface speed accessing/editing I/O files, and optimizations.
- SOMOS' fully automated processing speeds sequential running of multiple optimization actions.
- SOMOS' flexibility allows run restarts and result merges.
- SOMOS is being included within groundwater modeling packages such as Visual MODFLOW and Groundwater Vistas.

SUMMARY

SOMOS can optimize management of a stream-aquifer system for which the user has a calibrated simulation model. The general SOMOS release contains MODFLOW, MT3DMS and 14 optimization algorithms. Novice and accomplished optimizers both find SOMOS and its user's manual to be marvelous tools. They enable a relatively new modeler to compute optimal management strategies. They magnify experienced hydrologists in crafting magnificent strategies. SOMOS commonly yields 20-40% percent improvement versus using simulation model alone, but has yielded up to 58% improvement. SOMOS is being interfaced with powerful groundwater visualizers and modeling systems. A limited version is available at *http://www.usurf.org/units/wdl* .

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