

Introduction to Simulation/Optimization Modeling for Groundwater Contamination Remediation
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Normal use of a simulation model to develop a groundwater extraction/injection strategy employs the following process: (1) specify management goals, (2) assume a pumping strategy, (3) simulate system response to the pumping strategy, (4) evaluate acceptability of the system responses, (5) repeat steps (2-4) as required. This is a trial and error approach that is unlikely to actually yield the best pumping strategy for complicated problems.

Models are designed for a particular purpose. Simulation models are designed to predict system response to an assumed water management strategy. The user must input the pumping strategy before the model can do prediction. A different type of model is designed to compute the best pumping strategy for user-specified management goals and constraints. Such a simulation/optimization (S/O) model couples simulation capabilities with formal optimization algorithm(s) to calculate mathematically optimal pumping strategies.

Both normal simulation models (termed S models here) and S/O models require the user input appropriate descriptors of the physical system. The S model also requires the modeler to input a pumping strategy. The S/O model does not require that but does require the user input: (1) the objective function (ie. an equation the value of which the model should maximize or minimize--examples include the sum of pumping values, or the sum of installation, operation and maintenance costs); (2) upper and lower limits on acceptable values of variables (such as pumping, head, gradient, flow, concentration; and (3) other restrictions expressed as equations. Unlike a S model, a S/O model does not require input of a pumping strategy.

Optimization problems having linear objective function and all linear constraints are considered linear programming (LP) problems. Quadratic programming (QP) problems have quadratic objective function and linear constraints. Nonlinear programming (NLP) problems can have nonlinear objective function

Optimization problems range widely in complexity, required modeler expertise and computer computational effort required for solution. For simplicity, I here consider all three aspects when describing a problem as easy or difficult. The easiest problems are to minimize steady or transient pumping needed to create an obvious hydraulic barrier (recharge mound or extraction trough) when well locations are already known. Somewhat more difficult is computing a strategy that maximizes mass of contaminant removal or reduces concentrations to less than target levels (i.e. MCL) within a specified planning horizon.

Sometimes the user must select a set of potential well locations for the S/O model to consider in developing the optimal strategy. The S/O model will determine how much, if any, should be pumped from each potential well. This can add a level of difficulty because the modeler must rely upon experience and creativity to envision how the system might work--and then rely upon the S/O model to do the best it can with that vision.

It is generally more difficult to develop an optimal pumping strategy that assures capture by creating an obvious hydraulic barrier than one assuring capture via contaminant pathlines. This results because pathlines can curve and reverse direction 180 degrees within a capture zone. Assuring capture by pathline is also less robust than assuring it using obvious hydraulic barriers (there is less of a safety factor involved).

One of the more challenging problems computationally is to determine a least cost system design and installation to achieve cleanup and containment goals. The modeller must specify potential well locations and, in the most rigorous approach, the S/O model must consider the present value of installation, operation and maintenance costs of all combinations of pumping wells and rates.

One should remember that the S/O model will compute an optimal strategy for the problem posed by the modeler. If the modeler does not pose the right problem, or does not suggest the best potential well locations, the computed optimal strategy might be less optimal than a strategy computed for a differently posed problem.

Recall that different groundwater simulation models will often predict different water levels for the same location. Even different MODFLOW solvers can calculate heads that differ by several feet in regional problems. Similarly, depending on convergence criteria and solution approach, different

optimization algorithms can yield somewhat different answers for the same problem. This becomes more of an issue as problem nonlinearity increases. The more nonlinear the problem, the easier it is for the S/O model to present a locally optimal solution instead of the globally optimal solution. The more nonlinear problems involve transport as well as flow. The nonlinear flow of unconfined aquifers can be readily addressed by approximation methods so that flow optimization problems can be solved accurately using linear programming (LP) methods.

REMAX is by far the most powerful and user-friendly S/O model I am aware of. To perform simulation it can directly use MODFLOW (even with STR) and SWIFT. With existing utility programs it can be used with MT3D, ARMOS, QUAL2E, and other transport models to manage flow and transport in transient multiphase systems. REMAX simulation abilities also include: response matrix methods (perfect for linear systems and automatically adapted for nonlinear systems); response surface methods (polynomial functions and artificial neural networks).

REMAX optimization methods include classical derivative-based operations research approaches, branch and bound, and outer approximation, and alternative evolutionary approaches (genetic algorithm). It will solve a full spectrum of optimization problem types: linear (LP), quadratic (QP), nonlinear (NLP), mixed integer (MIP), and mixed integer nonlinear (MINLP). Its solvers are robust and widely tested.

Ramifications of Applying S/O Modelling to Groundwater Contamination Remediation, with Case Study Examples¹

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There are many consequences of employing simulation/optimization models while designing and while operating groundwater remediation pumping systems. Ramifications during the design phase can be discussed under the following topics:

(1) Calibration. One cannot optimize management of a system if one cannot adequately simulate system responses to management. A good calibration is important whether one intends to apply a normal simulation model (here termed a S model) or a simulation (S/O) model to subsequently develop a pumping strategy. If a contractor expects to be developing a plume containment strategy, he will likely apply greater pains during calibration than if he expects merely to be predicting future transport. Achieving good head and gradient matches during calibration is especially important if one expects to develop a containment strategy that must prevent a plume from crossing particular boundaries.

(2) Judgment. Assume one is developing a pumping strategy that requires the placement of new wells. It is very important whether using a S or an S/O model to use good judgment in placing potential well locations. Any S/O model practical for moderately sized well systems will only consider the well locations that one has told it to consider. Poor selection of potential well locations will result in a poorer optimal strategy than would result from wise selection.

(3) Tools. A S/O model is a better tool than a S model for developing a pumping strategy because it is designed for that task. S models require that the user input an assumed pumping strategy. A S/O model provides a better tool for computing the best pumping strategy for a particular situation. REMAX is the most powerful and user friendly S/O model I am aware of.

(4) Cost. Depending upon the complexity of the management problem, it might cost more money to develop a pumping strategy using a S/O model than using a S model. The benefit of S/O model application primarily results during and after construction. Then, it should result in reduced installation, operation and maintenance costs or in reduced contaminant concentrations. S/O models are not needed for simple problems. For example, a graphical approach is sufficient to determine optimal steady pumping from 3 wells applying only head constraints. By analyzing the results of many systematic batch transport simulations, one can also determine nearly optimal mass extraction pumping strategies for problems having three wells and steady pumping.

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(5) Monitoring Criteria. By selecting locations of head difference/gradient or concentration constraints to be used within the S/O model, one is beginning to identify the critical locations that should be monitored in the field. The earlier these are considered the better.

Ramifications during remediation system installation and operation can be discussed under the following topics:

(1) Cost. Assume the goal of the pumping strategy is cost minimization, subject to constraints. One would expect that such a pumping strategy developed via S/O model would cost less than one developed using a normal S model approach.

(2) Environmental Quality. Assume the goal of the pumping strategy is minimization of final contaminant concentration or maximization of mass removal, subject to other constraints. One would expect that a pumping strategy developed via S/O model would better achieve the goal than a strategy developed using a normal S model. Given modelling uncertainty this advantage is important.

(3) Reliability. Optimal pumping strategies developed by S/O model can be at least as reliable as those developed by simulation model alone. REMAX includes standard procedures for developing pumping strategies that are optimal and simultaneously satisfy constraints for multiple realizations (multiple sets of assumptions of aquifer parameters and boundary conditions).

(4) Feedback. Once a pumping system is installed and operated, pumping rates should be reevaluated periodically. Plume concentrations often do not change as models had predicted. Cleanup efficiency can be greatly enhanced by periodically adjusting pumping strategies to address changing plume conditions. Substantial benefits can result from doing this, even if using only simulation models. One would expect to derive even greater benefit from using a S/O model, although not as much as if one applies S/O modelling earlier in the remediation process.

Examples of employing S/O models for DOD sites that I have been involved with include the following:

(1) For one anonymous northeastern US site, a contractor asked me to develop an optimal pumping strategy to assure capture of a plume moving toward municipal wells. The strategy would involve pumping from industrial wells within the plume. The contractor had already developed a pumping strategy for this purpose using MODFLOW alone. Using REMAX I developed a pumping strategy that required 40% less pumping from the industrial wells. Furthermore, when the city later wanted to increase their pumping. REMAX easily computed the tradeoff curve showing the least amount of industrial pumping needed to keep the plume captured regardless of how much the city pumped. In another twist on this multiobjective optimization problem, the state water agency was concerned that too much groundwater pumping would cause excessive river dewatering and hurt downstream water users. By imposing an upper limit on total flow from river-to-aquifer, REMAX was able to compute (with only one additional optimization run) the optimal combination of pumping from municipal and

industrial wells that would best satisfy the goal. The final strategy included the maximum pumping the city could pump, plus the minimum the industry needed to pump to retain plume control, while not causing excessive river-aquifer interflow,

(2) At Norton AFB, the pumping strategy developed using S/O modelling via REMAX reduced 15 year system costs by \$5.8M, or about 22% from that developed using simulation alone.

(3) For a different Norton AFB site, an optimal strategy would require only two or three extraction wells (depending upon whether the contaminant source continues) instead of the five proposed by a contractor without using optimization.

(4) At Castle AFB, applying a REMAX-developed pumping strategy could reduce pumping by over 20%.

(5) At Wurtsmith AFB a pumping strategy that maximizes mass of contaminant removal is designed to immediately achieve plume capture and to achieve cleanup within six years.

In conclusion, how much benefit accrues from using a S/O model depends upon the problem, including how much freedom the modeler is given to develop the pumping strategy. If treatment facility capacity and well locations are already fixed and unchangeable, the S/O model is unlikely to give as much improvement as if there is more freedom in application. Similarly, the earlier in the remediation process one applies S/O modeling, the better.