RcP 228

REMEDIATION SIMULATION/OPTIMIZATION DEMONSTRATIONS

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ABSTRACT

Applications of simulation/optimization (S/O) software to develop contamination remediation strategies include formal remediation optimization using heads and gradients (hydraulics-based) and concentrations (risk-based) constraints. The six reported cases involve pump and treat systems, or pump, treat and re-inject systems, together termed PAT systems. We used S/O modeling to perform hydraulic optimization for two of the sites and transport optimization for four. For four of the six sites, other parties used normal simulation (S) modeling alone to develop pumping strategies. Comparing the S/O model-developed strategies with the S model-developed strategies showed S/O modeling benefits ranging up to: (a) 25 percent reduction in construction cost and 20 percent reduction in O&M costs; (b) 160 percent increase in mass removal; and (c) 62.5 percent reduction in number of extraction wells, and (d) 25 percent reduction in new wells with six percent increase in mass removal. The earlier that S/O modeling was used in the design process, and the more freedom given to the S/O model, the greater the benefit.

INTRODUCTION

S/O software has become increasingly powerful with time (Lefkoff and Gorelick, 1987; Geotrans, 1998; Ahlfeld and Riefler, 1999; HGS and SSOL, 2001. This paper describes some applications of S/O software developed primarily at the Dept. of Biological and Irrigation Engineering at Utah State Univ. Resulting optimal groundwater contamination remediation system designs have been built, or optimal management strategies have been implemented. Details are in a book to be published by DuPont Corporation.

A pumping (or management) 'strategy' is a set of spatially and perhaps temporally distributed water or chemical injection or extraction rates. A strategy can include 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 objective function, constraints and bounds. An optimal strategy developed for a specified 'scenario' is optimal for that scenario, but is probably sub-optimal for a different scenario. A posed scenario includes all assumptions required to specify the optimization problem and to apply the simulation model that the optimization algorithm needs to describe system response to management. Sometimes 'scenario' also refers to the strategy developed for a scenario.

The author and his students at SSOL[2] have designed optimal pump and treat or pump, treat and reinject (PAT) strategies or systems for several contaminated ground-water sites. For four sites the team used hydraulic optimization without transport optimization and for four they used transport optimization. They only used S/O models created by SSOL or HydroGeoSystems Group (HGS). These S/O models include flow and transport simulators, and algorithms for calculating optimal strategies.

The SSOL- and HGS-developed S/O models used operations research (OR) optimization and/or h euristic optimization (HO) algorithms. The OR algorithms used simplex, gradient search, branch and bound, and outer approximation to solve linear (LP), quadratic (QP), mixed integer (MIP), nonlinear (NLP), and mixed integer nonlinear programming (MINLP) optimization problems. HO approaches have included simulated

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annealing (SA), parallel recombinative simulated annealing (PRSA), and genetic algorithm (GA). SOMOS is our current modeling suite (Simulation/Optimization Modeling System)(SSOL, 2001).

A globally optimal pumping strategy is the best of all strategies that satisfy all constraints, (i.e. best within the feasible solution space). One can readily compute a globally optimal pumping strategy for LP problems. A locally optimal pumping strategy is better than all others within its part of the feasible solution space. Depending on the situation, any optimization algorithm can get stuck in a locally optimal solution.

Some groundwater remediation efforts emphasize cleanup (removing contaminant). Others emphasize containment (preventing contaminant from leaving a specified area). Some projects emphasize both goals. 'Capture' sometimes refers to either goal separately or both goals simultaneously.

One selects an optimization approach depending on the management goals and the available simulation model. In hydraulic optimization, one controls contamination by controlling heads and gradients. For this, S/O models do not need transport simulation module(s)--a flow simulation module suffices. Hydraulic optimization problems are generally linear for confined aquifers. Special SOMOS procedures allow it to also find globally optimal strategies for nonlinear (unconfined) aquifers (SSOL, 2001).

In transport (sometimes termed risk-based) optimization, one explicitly controls concentrations. To predict values of these usually nonlinear variables, S/O models include a transport simulation module. For nonlinear transport optimization problems gradient search OR techniques sometimes do not provide a sufficiently optimal strategy. For those problems SOMOS uses HO optimization.

The below two hydraulic and four transport optimization projects include cases in which: (a) PAT system hardware existed and no wells were to be added; (b) some PAT hardware was installed or scheduled for installation, and a pumping strategy existed, but additional hardware and were needed; and (c) all new wells were to be used in the optimal strategy. For four of the reported situations, another party had developed a strategy using a simulation model alone (referred to as an S model). If the S model-developed strategy was recent or simultaneous in time, I contrast that strategy with our optimal one.

EARLY PROJECTS INVOLVING S/O MODELING FOR PAT/PTR DESIGN

Optimizing Plume Containment at Norton AFB (NAFB)

This pump and treat optimization project was intended to contain a 4-mile by 1-mile TCE plume at the Norton AFB (NAFB), California, southwestern boundary. We used hydraulic optimization to design a PAT system and strategy to prevent the on-base plume portion from leaving NAFB. Another contractor developed a design for the site using the MODFLOW S model alone (McDonald and Harbaugh, 1988). We used LP to minimize total steady pumping subject to: (a) preventing contamination from crossing a n irregular base boundary or migrating to a lower stratum; (b) placing all wells on NAFB and trying to use two existing extraction wells; (c) restricting well extraction or injection based on aquifer characteristics; (d) assuring total injection equals total extraction; and (e) using an existing treatment facility if possible.

The Air Force Center for Environmental Excellence predicted our optimal strategy would save over 20 % in cost and over 30% in pumping (Peralta and Aly, 1995a). After our optimal desi gn was constructed, monitoring showed that it achieved the goals in the field--severing the plume at the base boundary.

Optimizing Pump Test Siting for Calibration and Minimizing Pumping to Contain TCE and PCE Plumes at March AFB (MAFB)

We used hydraulic optimization to aid site selections for pump tests and to design a PAT system and strategy for PCE and TCE plume containment (Hegazy and Peralta, 1997). The plumes extend for in a four layer fractured flow system. Regulators wanted to prevent further contamination from crossing the southeastern MAFB boundary. SWIFT (Reeves et al, 1986) was the background simulator (S model) for this system because it can employ dual porosities. We used draft simulation model parameters in our S/O model and LP to prepare reconnaissance optimal pumping strategies that identified areas where additional aquifer data was needed to improve SWIFT calibration. These guided new well installation. We minimized total steady pumping extraction from wells subject to: (a) preventing all 5 ppb and higher concentration groundwater from exiting the base in any layer; (b) placing all new wells on MAFB and considering existing wells as candidates for optimization; © preventing pumping at wells from exceeding sustainable rates; (d) permitting surface discharge of some treated water; (e) preventing ground water from reaching a landfill bottom; (f) using the existing treatment facility, if possible.

Wells were installed per our recommendations. The implemented pumping strategy is achieving plume containment in the vicinity of the designed system[3]. To complete containment along the MAFB boundary north of our area, the prime contractor added two more extraction wells tying these into the PAT system. In 1999 the containment system achieved the Operating Properly and Successfully (OPS) milestone.

Maximizing Dissolved TCE Cleanup at Central Base Area, Norton AFB, California.

We used transport optimization to create a steady PAT pumping strategy for cleanup of a dissolved phase TCE plume source area. Another contractor had prepared a PAT design and strategy (using MODFLOW and MT3D (S modeling techniques), which was being constructed while we were preparing our optimal strategy. One extraction well and the treatment facility were already installed. That contractor planned to install four additional extraction and four injection wells. Because all injection was to be distant from the plume, SSOL did not optimize injection—we used the uniform values of the other contractor. We assumed a three-year period and steady pumping and used gradient search nonlinear programming to maximize total TCE removal subject to (Peralta and Aly, 1995b): (a) applying upper bounds on total pumping; (b) applying upper bounds on pumping from each wells; (c) forcing total extraction to equal total injection; (d) preventing the concentration of flow entering the treatment facility from exceeding 150 ppb.

Comparison between our S/O-developed strategies and that developed by S modeling shows the benefit of using S/O modeling as early as practicable. Our optimal steady pumping strategy assumed there was no continuous TCE source. This two-well strategy would remove 160% more mass in three years than the five-well strategy developed by the other party. Our time-varying strategy assumed a continued TCE source, and required only three wells, instead of the five wells proposed by the other party.

Maximizing Dissolved TCE Cleanup at Mather AFB, California.

We used transport optimization to design a time-varying (transient) PAT strategy for TCE plume cleanup at the Mather AFB Aircraft Control and Warning site. The prime contractor had proposed steady pumping rates for 8 extraction and 8 injection wells, and a 270-gpm total flow rate to drop concentrations below 5 ppb within ten years. We used the same injection well locations and injection rates as the prime. We addressed scenarios differing in whether extraction pumping could change with time, and in whether we used the same extraction well locations as the prime (Peralta and Aly, 1996). We used gradient search NLP to maximize TCE extraction subject to: (a) bounding total flow; (b) bounding individual well pumping; and (c) forcing total extraction to equal total injection. When SSOL picked different well locations, our strategy required five fewer wells to remove eleven percent more than the S model strategy.

TCE and DCE Plume Containment and Cleanup near Mission Drive, Wurtsmith AFB (WAFB), MI

This case illustrates a phased approach for addressing uncertainty in management goals. It shows use of normal flow and transport simulation and hydraulic and transport optimization to create what might be termed an optimal pumping strategy. We designed a steady PAT strategy to cleanup and contain TCE and DCE plumes (Peralta and Aly, 1997; Aly and Peralta, 1997) using four phases. In phase one we performed random simulations to try to identify the most suitable objective function and constraints for

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[3] *Personal communication, Olav Johanneson, EarthTech*

cleanup (transport) optimization. We evaluated: (a) minimizing present worth of installation, pumping and treatment costs; (b) maximizing removal of TCE plus DCE mass; (c) minimizing the sum of the greatest residual concentrations of TCE and DCE. Then we proposed an optimization problem formulation.

In phase two, we used a GA and artificial neural network (ANN) in transport optimization to develop a strategy that maximized TCE mass removal subject to: (a) causing TCE and DCE concentrations to drop below 94 and 230 ppb, respectively, within 6 years; (b) limiting total pumping to less than treatment plant capacity; (c) applying a 400 ppb upper limit on blended TCE and DCE concentrations; allowing surface discharge of treated water; assuring individual well pumping is sustainable. In phase three we used LP hydraulic optimization. We minimized the extra pumping (in addition to that determined by phase two) needed to contain the TCE and DCE. In phase four we manually changed the previously developed strategy to create a quasi-optimal strategy. We manually increased pumping rates up to the treatment plant capacity to yield a set of strategies ranging in cost and speed of cleanup.

RECENT S/O MODELING FOR PTR DESIGN

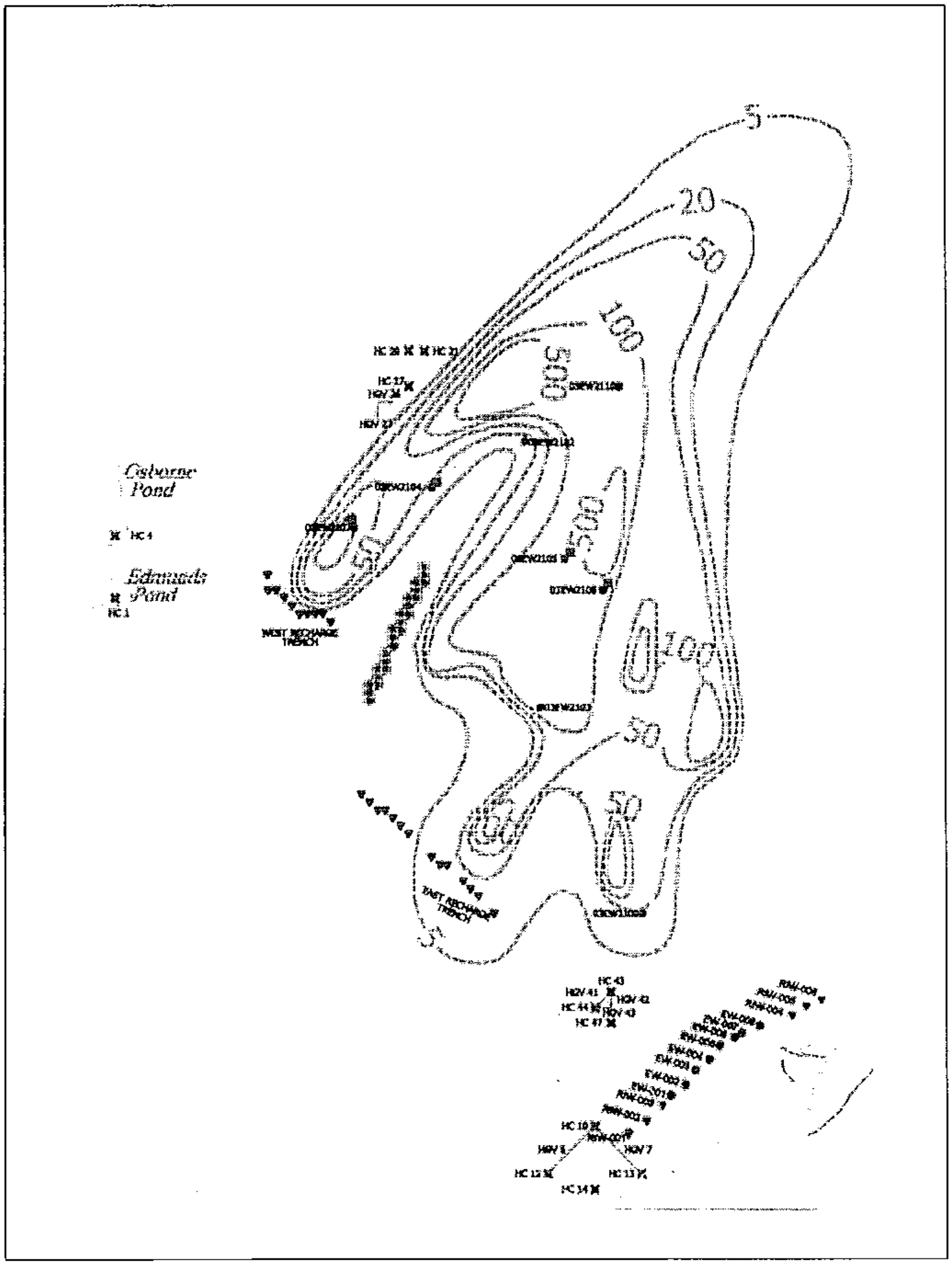
A recent transport optimization example illustrates optimizing PAT system and strategy design for cleanup and containment of the Chemical Spill 10 (CS-10) TCE plume on Massachusetts Military Reservation (MMR). The three-lobed plume is three miles long and one mile wide (Figure 1). It sinks to 200 feet beneath sea level in a glacial outwash composed primarily of coarse- to fine-grained sands, with discontinuous deeper silt and clay layers. Hydraulic conductivity generally ranges from 150 to 290 ft/day.

An Interim Record of Decision required: (a) capturing the plume's leading edge; (b) progressing towards cleanup; and (c) protecting the ecosystem, and previously clean water. A prime contractor had developed a PAT system and strategy using MODFLOW and MT3DMS in 21 layers, 118 rows, and 114 columns. The prime had installed or sited 13 extraction wells, 6 injection wells, and 2 injection trenches. The prime was considering system improvements, which led to its draft pumping strategy Run57. Run57 involved: adding an extraction well to prevent the western lobe from smearing to the east and contaminating clean aquifer; (b) adding an extraction well north of Sandwich Road (SR) to reduce the time the SR wells will pump; (c) adding an extraction well up-gradient of the northernmost existing well to reduce total cleanup period duration (d) possibly adding a well to the northwest to aid cleanup and containment.

HydroGeoSystems (HGS), supported by SSOL, was also tasked with making recommendations for system enhancement (HGS, 2000). The combined HGS-SSOL team is referred to as SSOL. After evaluation, SSOL generally concurred with the prime contractor's approach. Then SSOL maximized 30-year TCE extraction from nine in-plume wells plus SR wells, subject to: (a) preventing more than 0.5 feet of head change in Edmunds and Osborne Ponds; (b) preventing 5 ppb or greater concentrations from crossing the MMR boundary and from migrating from the western lobe to the southwestern lobe; (c) preventing total extraction at in-plume wells from exceeding 2700 gpm; (d) forcing total extraction at eight Sandwich Road wells to equal that of Run57; (e) forcing total recharge at West and East trenches to equal total extraction from eight in-plume wells; (f) forcing total injection at Sandwich Road injection wells to equal total extraction at the eight Sandwich Road extraction wells; (g) restricting pumping at individual wells so as to not exceed limits based on line, pump and well sizes; (h) applying loose head or head difference constraints at the U.S.G.S. research site and the LF-1 plume.

SSOL developed different pumping strategies for different assumptions. SSOL recommended using an eight-well optimal strategy. Simulation predicted that implementation for 30 years will extract about six percent more mass than Run57, require 50 gpm less extraction, and satisfy all constraints. (A SSOL-developed time varying pumping strategy using those wells would be yet more cost-effective).

Figure 1. MMR Chemical Spill 10 plume, model grid, constraints and optimal pumping locations (from HGS and SSOL, 2000).



With minor adjustments, the proposed wells have been constructed. Optimization aided well placement and will enhance mass removal, probably shortening cleanup duration. Benefit was less than it might be otherwise because: (a) the pumping strategy had to satisfy conditions outside the CS-10 modeled area (these conditions could only be evaluated by other models after strategy development); (b) plume cleanup would not be possible within 30 years due to fiscal constraints and contaminated silt layers; (c) the PAT system was already partially installed; and (d) the optimization problem was very constrained. Nevertheless, the S/O-model derived strategy and design showed benefit and was constructed.

CONCLUSION

S/O modeling yielded better PAT designs than those developed using only simulation (S) models. The earlier that S/O modeling was used during design, the better. One can expect a twenty percent improvement in remediation, pumping rate, or cost if using optimization. However, the benefit depends on the scenario, optimization objective, how much freedom is allowed to optimize, and other factors.

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APPENDIX A. SOMOS OVERVIEW

SOMOS (Simulation/Optimization Modeling System) is the evolving product of over five generations of different approaches to groundwater management optimization. The SOMOS groundwater optimization modules most pertinent for this paper are SOMO1 and SOMO3. Each module: (a) utilizes well-known simulation model(s) to predict hydrogeologic system response to stimuli; and (b) employs optimization algorithms to develop the best water management strategies for a posed management problem.

SOMO1 uses the porous media MODFLOW ground-water flow, including the STR stream flow package (Prudic, 1989), to describe flow. SOMO1 develops discretized convolution integrals that substitute for MODFLOW in the optimization process. To predict contaminant transport, SOMO1 can use polynomial equations developed from outputs of any other simulation model. [4] SOMO1 uses powerful optimization algorithms to solve linear, nonlinear, mixed integer, and mixed integer nonlinear optimization problems.

The developmental SOMO2 uses SWIFT, a fractured media simulation model, and the same optimizers as SOMO1. SOMO3 uses MODFLOW and MT3DMS to simulate flow and transport and to help train its artificial neural networks. SOMO3 uses heuristic optimization alone, or coupled with artificial intelligence.

SOMOS or its precursor modules have been well proven in real-world projects. SOMOS is designed for use by consultants, students, academics, and agency personnel. It can be readily applied to complex plume problems. Its powerful optimization and artificial intelligence modules will improve user satisfaction with developed strategies. It can help increase water use, protection, and cleanup and reduce cost.

[4] *One can develop the polynomials by statistically analyzing many simulations. Ejaz and Peralta (1995a,b) developed polynomials to predict surface-water pollutant concentrations. They applied these to optimally coordinate ground water and river water use or pollutant loading. Cooper et al (1998) made polynomials describing non-aqueous phase liquids (NAPL). They optimized floating petroleum management*