PROJECT COMPLETION REPORT

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Title: Augmentation of Optimal Management Policy Selections
to Groundwater Contaminant Transport Model MT3D, I and II

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Abstract:

The groundwater quality and management problems are concerned issues for practically every sector of the society. Efforts must be made to protect surface and ground water from degradation and to better manage such natural resources for greater social benefits. Due to intrinsic complexity and technical difficulties of dealing with groundwater problems, modeling efforts are widely exercised and greatly appreciated. As our federal government budget for water resources research and management struggles year after year and the cost for managing groundwater resources and for developing new groundwater technologies continuously increase, good reliable computer models become more essential for finding cost-effective groundwater management policies and best remediation designs. Existing publicly available computer codes only help identify such best strategies in steady state situations of small sizes or in a limited number of field conditions. We developed a framework for designing optimal pump-and-treat remediation systems and other optimal management policies. The framework consists of two optimization algorithms augmented to two existing popular simulation codes MODFLOW and MT3D in the form of computer software. Our initial version of computer software consists of two separate packages (MT3DOPT and DOMODF) based on two completely different types of optimization strategies. They are capable of combining the expert knowledge of good management policies and reasonable remediation designs with the effectiveness of optimization oriented search techniques. Our models can be used as guiding tools for a wide variety of users to identify better strategies to save a considerable portion of huge remediation costs under existing technologies and to find better policies to achieve groundwater management objectives.
Problem and research objectives:

Managing groundwater resources is a political, scientific, and social issue of our society. How to effectively protect, utilize, or remediate such natural resources is one of the frequently asked questions in the groundwater community. In particular, groundwater contamination has been a serious environmental problem in the United States for many years. Because of slow groundwater movement in the subsurface environment, and because of the complex interaction between contaminants and geological surroundings, remedial actions designed to clean up contaminated groundwater at a given hazardous waste site can last decades and cost hundreds of millions of dollars (e.g., DOE(1988); EPA(1992)). Even a cost reduction by a small fraction could mean a significant amount of savings.

While many new technologies are emerging for in-situ remediation of contaminated groundwater, pump-and-treat is still by far the most prevalent technique for groundwater remediation (e.g., EPA(1992). Even in hazardous waste sites where alternative remediation techniques (such as bioremediation) are implemented, a pump-and-treat system is often installed to supplement other remediation processes. Pumping is also widely regarded as a critical part of decision making in other groundwater management problems. But it does not seem to be obvious at all regarding how to identify the best well locations and the best pumping-injection rates by the trial-and-error method without using any optimization oriented search techniques. Given the countless number of possible designs, the trial-and-error process is understandably tedious, and after all there is no guarantee that it will result in an optimal design within a reasonable time frame. Given the large number of hazardous waste sites and the huge remediation costs that are expected to more than triple from $3.4 billion in 1992 to 11.2 billion by 1999 (see NGWA(1993)), it is obviously of significant economic benefit to develop an optimization-simulation model that can be used to help identify the most cost-effective groundwater remediation scenario. Likewise, an optimization-simulation model will also help identify an optimal strategy for other groundwater management scenarios such as the groundwater supply problem. Researchers have been actively studying the use of optimization techniques for pump-and-treat remediation designs and other management decision making in recent years (e.g., Gorelick(1983); Gorelick et al.(1984); Harvey et al.(1994); Ahlfeld et al.(1988); Andricevic and Kitanidis(1990); Culver and Shoemaker(1992), Wagner(1995), Rogers et al.(1995)). While significant progress has been made in research on optimization of groundwater policy designs with several optimization-simulation packages reported, public consumption of those results seems to be limited either because of the restriction of the simulation component of the codes or the optimization procedures used in the codes.

The main objective of this two year project is to develop an initial version of a new alternative framework for designing optimal pump-and-treat remediation systems and other optimal management policies for the purpose of a wider range of public consumption. The framework consists of optimization algorithms augmented to existing popular simulation codes MT3D(cf. Zheng(1990)) and MODFLOW(cf. McDonald and Harbaugh(1988)) in the form of computer software. It is capable of accepting expert knowledge of good management policies and reasonable remediation designs as a part of its input data files and improving such input policies through guided search processes. Our model can be used as a guiding tool for its users to identify better strategies to save a considerable portion of huge remediation cost under existing technologies and to find better policies to manage groundwater resources.
Major activities and methods:

Our project duration is from June 1, 1994, to May 31, 1996 for two years. The first year is limited to developing a theoretical framework and a basic integrated program package with limited testing on hypothetical examples. Our second year's effort is devoted to development of the second package and more testing which results in various refinements of our basic program packages.

We have investigated two types of optimization algorithms. One of them is static, based on the genetic algorithm (GA). The other is dynamic, based on the differential dynamic programming method (DDP). In order to benefit the public as much as possible, our optimization algorithms are integrated into two existing popular groundwater simulation codes. The first optimization algorithm is augmented to a modified version of the widely used three-dimensional contaminant transport simulation model MT3D to create an optimization-simulation model for determining optimal well locations and pumping-injection rates under a variety of field conditions. The resulting package is called MT3DOPT. The second one is augmented to a modified version of MODFLOW. The combined code package is referred to as DOMODF. The combination of existing popular finite difference simulation codes and optimization-optimal control methods is a unique feature of our methodology.

In order to effectively link our optimization procedures with MODFLOW and MT3D, we had to restructure these two codes and designed some linkage programs. A considerable portion of project time was devoted to this task. A number of examples have been tested with our programs, which is another time consuming task of the project. The examples cover a variety of scenarios, including all the possible dimensions of aquifer domains, different objective functions and constraints that are commonly encountered in practical applications. In addition to hypothetical examples, we used two superfund examples for further verification. Several of those examples and their testing results are included in the attachments of this report.

Our other approach for solving the problem we have proposed is to find analytical optimality conditions for the original continuous problem (continuous state and continuous time) before discretization. We have investigated analytical conditions of optimality by using a Volterra-Picard series for representing the solution of the continuous version of the problem.

During the course of project, several students had been involved and benefited in different ways. Mingguang Wang, a new Ph.D. student transferred from Pennsylvania State University, has worked on this project with over 75% of support provided by this project. It is expected that our research results will lead to an important part of his Ph.D. dissertation. There were two undergraduate students, Erin Akin and Amber Jenkins, and three other graduate students, Dan Altenburg, Yaodong Wang, and Wei Li, who worked on numerical algorithms related to this project. Y. Wang and W. Li did their master degree's projects in this area. Results of this project have been partially integrated into the groundwater modeling course offered by the Geology Department at the University of Alabama.

Principal findings and significance:

We found that both types of optimization algorithms work in principle for problems with single or multiple management periods. However, the GA version is more suitable for problems with single or a small number of management periods, while the DDP version is much more powerful in dealing with a larger number of management periods. However, the DDP version is
more error sensitive since it requires derivatives derived from the objective function, constraint functions, and the state equation. Since the contaminant transport equation is highly nonlinear, we adopted only the GA option for the transport model in the current version, while both GA and DDP options are available for the flow model.

Existing groundwater flow and contaminant transport simulation models (MODFLOW and MT3D respectively) were originally designed for a single simulation run. In our project, they are restructured in order to be effectively incorporated into our optimization methods. With the differential dynamic programming, the sensitivity calculation is the most time consuming task. It is also a major suspected source of numerical error and instability. We have designed several options to partially overcome such potential problems. However, we found that additional work would be needed to effectively link our dynamic optimization method to the transport model.

Our testing results with both algorithms show at least local convergence and significant improvements over reasonable trial-and-error results. As our field examples have indicated, optimization oriented search methods generally result in much better policies than what an experienced groundwater professional can get by the trial-and-error process. One is referred to the attachments of this report for more detailed results.

We also investigated several other numerical algorithms that might potentially be incorporated into our optimization-simulation models for future upgrades. In addition, we have found some analytical optimality conditions for the original continuous problem, which could also eventually lead to numerical schemes for finding an optimal management strategy. Such upgrades will be made subject to availability of future funding.

Most findings of this study have been presented at a number of professional conferences and published in their proceedings. Additional papers or presentations may follow. This study as well as studies conducted by other researchers indicates that the combination of optimization and simulation is a sensible approach for designing optimal groundwater management policies and pump-and-treat remediation processes. The dynamic optimization approach is particularly powerful in dealing with problems involving a large number of flexible management periods, in which case static optimization algorithms are likely to become practically infeasible. Our dynamic optimization code DOMODF is an attractive tool for solving such long term decision making problems in groundwater modeling. Optimization and simulation together do save time, effort, and money. Our programs can be used by polluting industries and waste management firms and their consulting partners to design better waste disposal systems and desirable remediation strategies. They can help environmental agencies at different government levels to regulate and monitor groundwater remediation processes and to better manage groundwater resources for greater social benefits.

Although our mathematical models and computer codes won't replace groundwater technologies, they can be combined with existing technologies. They provide efficient, convenient, reliable, and cost-effective means to help (a) protect groundwater from degradation, (b) study the fate and transport of contaminants in the ground water, (c) design good groundwater remediation strategies, (d) save a considerable portion of huge remediation cost under existing technologies, (e) identify desirable groundwater management policies. Our programs are designed in such a way that individual users just need to prepare regular MODFLOW/MT3D input data files plus an additional problem specific input file in order to solve a particular optimization problem. Several sample files are provided in the attachments of this report. In a lot of cases, the user just needs to slightly modify the sample files before a particular run. More detailed instructions regarding the use of our computer codes are also provided in the attachments of this report.
Publications and professional presentations:

Belbas, S.A. "Continuous and impulsive optimal control of Goursat systems", invited lecture at the Fifth International Colloquium on Differential Equations, Plovdiv, Bulgaria, August 1994.


Belbas, S.A. "Optimal control of Goursat systems over general domains", presented at the Sixth International Colloquium on Differential Equations, Plovdiv, Bulgaria, August 1995.

Belbas, S.A. "Forward dynamic programming for numerical solution of optimal control problems for parabolic systems", to be presented at the Seventh International Colloquium on Differential Equations, Plovdiv, Bulgaria, August 1996.


Wang, M., C. Zheng, and M. Sun, Simultaneous optimization of pumping rates and well locations in capture zone design, presented at 1996 Spring Meeting of American Geophysical Union, Baltimore, MD. Its abstract is published in the conference proceedings.

Zheng, C. and J.J. Jiao "Theory and application of a three-dimensional contaminant fate and transport model", Presented at the 1995 Southeastern Regional Meeting, Geological Society...
Conclusions:

Despite of very limited level of funding for this two year project, we have produced two packages of optimization-simulation codes to help design optimal groundwater management policies and pump-and-treat remediation processes. We demonstrated with a number of examples that the combination of optimization and simulation is a sensible and cost effective approach for solving various decision making problems concerning groundwater resources under currently available technologies. Since our computer codes are based on two widely used groundwater simulation codes MODFLOW and MT3D, they can be easily adopted by a large number of groundwater researchers and practitioners. Our investigation also revealed needs for future improvements. We intend to upgrade our codes based on our continuing work in this direction. At this stage, we advise anyone who is interested in using our new computer software to contact us directly for a complimentary copy of demonstration software.

References:

Department of Energy (DOE), 1988, Site-directed subsurface environmental initiative: five-year summary and plan for fundamental research in subsoils and groundwater, Rep. DOE/ER-03344/1, USDOE.

Attachments:


B. Optimal Remedial Policy Selection Under General Conditions, A brief user's guide to MT3DOPT.