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DEVELOPMENT OF A COMPREHENSIVE MODELING SYSTEM FOR REMEDIATION OF CONTAMINATED GROUNDWATER

by Jeffery P. Holland¹, A.M. ASCE

Abstract

The U.S. Army Engineer Waterways Experiment Station (WES) has proposed development of a Groundwater Modeling System (GMS) for simulating groundwater flow, the transport/fate of subsurface contaminants, and the efficacy of remedial actions. The GMS is proposed to support the needs of the U.S. Army in three main areas: site characterization, contamination assessment, and evaluation of remediation alternatives. To do this, the GMS will include numerical algorithms for simulating the hydrogeologic and biogeochemical processes that must be considered when developing remediation programs for Army and other sites. An essential feature of the GMS will be user interfaces which augment model application and visual presentation of results. The GMS project will include a strong technology transfer element that will instruct engineers and scientists in its capabilities and use.

The primary product from the proposed research will be a three-dimensional modeling system centered around both single and multi-phase flow in concert with single and multiple-component groundwater contaminants. The system will be capable of simulating flows in both the saturated and unsaturated zones. Although the system will be keyed to the specific requirements of the Army, the system will also be formulated in a fashion general to support its use by others. Partnering with other Federal agencies will be established as appropriate as a means of extending the range of applicability of the proposed modeling system.

Introduction

Groundwater is the major source of water supply for over 50 percent of our population. This precious resource is threatened by increasing amounts of contamination. The variety of pollutant sources and their characteristics compound the problems associated

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with groundwater contamination detection, control, and cleanup. The U.S. Environmental Protection Agency (EPA) has stated that the most serious threat to human health and the environment is contaminated groundwater. Activities at military installations have produced contamination of groundwater which may pose problems for human health and may threaten wildlife habitat and wetlands adjacent to or on these posts. Over 10,000 U.S. Army sites were originally identified as having the potential for hazardous and toxic wastes (HTW) concerns; approximately one-half of these are still under investigation or will require some level of remediation (Department of Defense, 1991). In fact, the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) has indicated that the Army is spending more on groundwater-related problems than any other cleanup activity at Army installations. For example, at the Rocky Mountain Arsenal approximately \$315 million had been expended on remediation-related efforts through the 1990 fiscal year (Department of Defense, 1991).

Mitigation of contaminated groundwater is a difficult problem because the contaminants exist in complex hydrogeologic conditions where a variety of physical, chemical, and biological processes are occurring. Multiple sources and sinks of water and contaminant exist. Multiple fluid phases and contaminant states are common to HTW sites. A wide variety of contaminants, ranging from non-aqueous phase liquids (i.e., petroleum hydrocarbons and organic solvent liquids) to heavy metals and explosives residues is present on Army installations. The ability to determine the extent and severity of contamination is required before groundwater investigations can rationally proceed from the preliminary assessment phase into the investigation and implementation of various remedial measures. Iterative or unfocused remedial actions are unacceptable when human health, safety, and costs are considered. Therefore, one must have the capability to evaluate the effectiveness of alternative remedial measures prior to their selection and implementation.

Much of the information required for development and evaluation of economical and effective remedial measures can be obtained using computer models. Numerical groundwater models have been developed that address specific problem areas such as flow, infiltration or recharge of groundwater, contaminant transport, dilution of contaminant, and groundwater removal (Environmental Protection Agency, 1988). However, a truly comprehensive groundwater model which adequately addresses all important aspects of contaminated groundwater flow and transport is needed to support remediation activities.

Needs for the GMS

Given the above statements, generalized groundwater modeling tools, such as the GMS development proposed, are needed for a variety of reasons including: (a) to lessen the burden of the enormous costs expected in contaminated groundwater cleanup; (b) to allow improved assessment of temporal and spatial effectiveness of remedial actions;

(c) to provide a mechanism for understanding and integrating multiple flow and contaminant processes; and, (d) to produce a methodology for assessment of the sensitivity of remedial measure effectiveness to key geophysical and biochemical parameters. Ultimately, of course, the true need for the GMS, and the proof of its concept, is in the improved design of more cost-effective and efficient remedial measures, and as an aid to site characterization.

Technology and Knowledge Gaps and Barriers

A variety of technical gaps will be, in part or total, overcome as a part of a development of the type envisioned above. These gaps have been delineated in part by several (see, for example, National Research Council, 1989). The major of these gaps relative to the concerns of the U.S. Army include:

- * Unsaturated zone modeling is in its infancy
- * Fracture-flow interaction processes are poorly understood
- * Multiphase flow and multi-component contaminant modeling require extensive additional development
- * Spatial heterogeneities, especially in three dimensions, are poorly represented numerically
- * Limited, or no, information on a host of fundamental contaminant transport processes is available
- * Little information on the temporal aspects of remediation scheme design/operation exists
- * Relatively-friendly numerical models having greater applicability for a variety of site-specific cases are generally unavailable

Technical Approach

Development of the proposed generalized groundwater modeling system is envisioned as a six-year, highly integrated effort. While the effort will focus on key aspects of the remediation of contaminated groundwater resources at Army installations, engineering aids for site characterization and contaminant assessment will also be developed. Central to the effort will be the development of three-dimensional, time-varying groundwater flow and contaminant transport models capable of both short-term and long-term simulations. The major components of the GMS as proposed are as follows:

- (a) site characterization tools, including data base managers, visualization software, and screening-level tools in the form of analytic and simplified numerical groundwater flow and solute transport algorithms. These will be coupled to a graphical user interface to form the backbone of the GMS. Guidance, in the form of manuals and knowledge-based systems, will also be developed to provide information on the utility of existing models for characterization and remediation evaluations. Additionally, methods for estimating geophysical

parameters will be developed. These methods will couple visualization, estimation mathematics, guidance on field data collection and sampling, and some aspects of uncertainty analysis to aid site engineers.

(b) contaminant assessment and transport tools, including two and three-dimensional groundwater flow and contaminant transport models. These models will simulate time-varying conditions in the coupled saturated and unsaturated zones for a variety of common, and several military-unique, contaminants. These models will be coupled with the GMS framework mentioned above. Single-phase and rudimentary multiphase flow simulation capabilities will be incorporated in the system. Single-component, and some multiple-component, contaminants will be simulated at this level.

(c) tools to simulate the efficacy of various remediation methodologies for cleaning up site-specific sites. These tools will be tailored to simulate the most attractive remedial treatment technologies such as (but not limited to): pump and treat, bioremediation, physical containment, steam injection, etc. Other methods may be added as appropriate, given that this field is changing rapidly. Additionally, this level of simulation would provide the user with optimization capabilities for the design and operation of various treatment technologies (such as provision of the optimal number and location of pumping and injection wells). Uncertainty and risk will also be built into the system to allow for incomplete site characterization (i.e., sparse field data, poor parameter estimation, etc.) and/or poor process understanding.

To provide the products alluded to above, the GMS will be developed under seven highly integrated areas: site characterization, numerical simulation of physical processes, numerical simulation of contaminant processes, numerical simulation of remediation alternatives, user interface and visualization development, code verification, and technology transfer.

Deliverable Products

Given below is a listing of the major products, and their proposed delivery dates, to be developed within this investigation. This table assumes a FY92 start date for all requested funds for this program.

<u>No.</u>	<u>Product</u>	<u>Delivery</u>
1	Refined scope of Army needs	FY92
2	Evaluation of groundwater modeling state-of-the-art	FY92
3	Documentation of Army requirements for GMS	FY92
4	Guidance on use of existing multi-dimensional groundwater models	FY93

5	Initial visualization and parameter estimation tools and guidance	FY93
6	Initial GMS for flow with user interface	FY93
7	Initial calibration/verification of GMS	FY94
8	2D,3D single component contaminant modules	FY94
9	3D flow module with rudimentary multiphase capabilities	FY94
10	Demonstration of GMS for selected field application	FY94
11	Improved multiphase constitutive equations	FY95
12	Enhanced GMS interface	FY95
13	Addition of improved multiphase compartments to GMS	FY96
14	Addition of multi-component compartments	FY96
15	Further verification of GMS via lab and field data	FY97
16	Completion of GMS and full documentation	FY97
17	Additional demonstration of GMS components for selected field site(s)	FY97
18	Technical workshops on use of GMS	FY97+

A component of the products listed above that should not be lightly overlooked is the calibration/verification phase of the GMS development. Calibration and verification are of importance in the development of any numerical model of physical processes, but these two activities are doubly vital for the GMS development. The credibility of the proposed development, both within the Army and to the outside technical community, is fundamental to the system's acceptance by regulatory agencies and, thus, its use. Further, putting regulatory issues aside, the system must properly simulate the individual physical processes which it integrates. Failure to do so may result in the design of remediation measures that operate properly for a few years and then decline in effectiveness. Thus, very rigorous calibration/verification actions are planned. These actions include comparison of model predictions with laboratory and field data (again leveraging previous efforts for these data where possible) for cases of ever-increasing sophistication. Further, in addition to technical reports, peer-reviewed papers will appear in notable technical journals to allow open critiques of the process and numerical formulations used to build the GMS.

Aspects of GMS Development Strategy

The current rate of development in the area of groundwater flow and contaminant transport modeling is both fast and furious. The expected investment required to conduct the research above, when coupled with the extensive number of technical gaps that must be tackled in the research, requires that current and near-future research be leveraged effectively. In an effort to do just this, WES has sought to develop partnerships with several federal agencies who are currently conducting research in contaminated groundwater cleanup: EPA, the Department of Energy, and the U.S. Geological Survey. Additionally, WES is partnering with the U.S. Army Toxic and Hazardous Materials Agency to maximize the effectiveness of the proposed research in meeting the needs of the Army user community,

and in transferring the products of the research to said community.

WES is actively seeking the advice of the National Research Council's Water Science and Technology Board (WSTB) to: (a) ensure that the current state-of-the-art in groundwater modeling is fully illuminated; (b) aid WES in scoping the actions that can be conducted over the next three to ten years to advance that state-of-the-art; and (c) delineate the abilities of the products of those actions to meet the needs of the Army.

Conclusions

The Waterways Experiment Station has proposed the development of a comprehensive groundwater modeling system for use in the cleanup of contaminated groundwater resources at U.S. Army sites and installations. In conjunction with USATHAMA and Headquarters, U.S. Army Corps of Engineers, WES is continuing refinement of the effort's initial scope. The modeling system will be designed to aid the Army in the areas of site characterization, contaminant assessment, and remedial treatment alternative design and operation. The proposed six-year research effort will seek to strongly leverage ongoing and near-future research by other groups through partnering with several federal agencies and universities.

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