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Project Summary

Compilation of Saturated and Unsaturated Zone Modeling Software

(Update of EPA/600/R-93/118 and EPA/600/R-94/028)

Paul K.M. van der Heijde

The full report contains the results of the evaluation of the capabilities of a large number of ground-water software packages designed for simulating flow, and transport and fate processes in the saturated and unsaturated zone, and for analyzing related ground-water management problems. Specifically, the evaluation and description of the software are presented in terms useful to determine applicability to ground-water protection and remediation problems. The results of this work are intended to serve as a first-level screening tool when selecting software for a particular application.

The study reflects the ongoing ground-water modeling information collection and processing activities at the International Ground Water Modeling Center (IGWMC). The full report provides an update to Compilation of Ground-Water Models by P.K.M. van der Heijde and O.A. Elnawawy (EPA/600/R-93/118, May 1993). The previous report presented a methodology used by the International Ground-Water Modeling Center (IGWMC) to classify, evaluate and manage descriptive information regarding ground-water modeling codes for the purpose of model selection. This methodology is implemented in the MARS (Model Annotation and Retrieval System) database. The current report presents an updated retrieval of information, and provides a more inclusive and current description of both saturated and unsaturated zone models included in the MARS database. Unsaturated zone model descriptions have been updated from Identification and Compilation of Unsaturated/Vadose Zone Models (EPA/600/R-94/028, March 1994).

The full report briefly discusses the information acquisition and processing procedures, the MARS information database, and the preparation of information tables. But the major significance of the report is an update of the appendices of the aforementioned reports. Appendix A provides cross-references between the unique database record identification number (*i.e.*, IGWMC Key), the name, title, or acronym of the software, and the authors. Appendix A also refers to the detailed description of each program as provided in Appendix C. Appendix B provides an overview of the software, organized by software category or type. The information in this appendix is cross-referenced with other appendices through the program name and IGWMC Key. Appendix C includes detailed information on each program's author and institution of development, the code custodian, level of documentation, verification and peer review, and if it is proprietary or in the public domain. Furthermore, each description includes a summary of the purpose of the program, the processes it may

simulate, the general mathematical method employed (boundary conditions and solution methods), output options, and user interface information. Finally, Appendix D contains pertinent references sorted by IGWMC Key, while Appendix E is a cross-referenced table for the software distributors.

This Project Summary was developed by EPA's Subsurface Protection and Remediation Division, National Risk Management Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at the back).

Introduction

The full report contains the results of the evaluation of the capabilities of a large number of ground-water software designed for simulating flow, transport and fate processes in the saturated and unsaturated zone, and for analyzing related ground-water management problems. It consists of a brief discussion of research approaches, and tables containing detailed information regarding more than 500 ground-water modeling programs. This report provides an update of information contained in the appendices of the reports, "Compilation of Ground-Water Models" (van der Heijde and Elnawawy, 1993) and "Identification and Compilation of Unsaturated/Vadose Zone Models" (van der Heijde, 1994(a)).

Ground-water modeling is a computer-based methodology for quantitative analysis of the mechanisms and controls of ground-water systems, and for the evaluation of policies, actions, and designs that may affect such systems. Ground-water models range from complex, resource-intensive, predictive or recursive research tools to practical, problem-solving tools. Most models are based on mathematical descriptions of physical, chemical, and biological processes active in a ground-water system, and on the causal relationships among selected components of that ground-water system. Many of these models focus on single-phase fluid flow in the saturated and/or unsaturated zone and the migration of dissolved constituents. Other models provide for analysis of multi-phase fluid flow and the complex chemical processes and phase transfers that might take place in such systems.

In recent years, sophisticated general-use software, and powerful desktop computers and workstations have come within reach of many ground-water professionals, facilitating extensive data management, complex simulations, in-depth pre- and post-simulation analysis, and enhanced graphic display. These technological innovations have a significant impact on the analysis of ground-water problems and the preparation of ground-water -management decisions. Moreover, in recent years the ground-water profession has seen a rapid increase in scientific research regarding the physical, chemical and biological processes active in the subsurface, the mathematical theories to describe these processes, and techniques and methodologies to characterize field systems and the uncertainty in such characterizations. As a result, computer-based decision-support in ground-water management has taken the form of integrated software solutions for particular types of management problems, where various data management, analysis and display tools are interwoven and embedded in a generic or problem-type, dedicated, user-friendly computer interface.

To manage the information on such a wide variety of software, the International Ground Water Modeling Center (IGWMC) developed a new version of its ground-water modeling software information database MARS (Model Annotation and Retrieval System; van der Heijde, 1994b). This database is designed to accommodate information regarding software for ground-water simulation, geostatistical analysis, model input preparation, postprocessing of simulation results, and various types of advisory systems. As of September 1994, this database contains, more than 800 software descriptions.

Information Acquisition and Processing Procedures

The initial information on ground-water modeling software comes from the review of open literature, from presentations and discussions at conferences, workshops, and other meetings, and directly from researchers and software developers. Once a software item of interest has been located, additional information is collected from the team that developed the software, and from pertinent literature. The collected information is used to update the MARS referral database. In selecting a software item for inclusion in this database, special attention is given to the importance of the software for practical applications, and to its development status (*e.g.*, research tool or deliverable versus generally applicable, well-tested and documented routine tool). Other considerations for inclusion in the database are prominence of the software name or acronym, importance of software for research, and reputation of software development team. Descriptions of the software's concepts and mathematical framework are found in peer-reviewed literature and in the software documentation. Operational characteristics, computer requirements, and information on the level of testing to which the software has been subjected, are taken from the user's manual, if available.

The MARS database was initiated in 1991. The result of the first phase of the project was a database of about 500 records, which served as the basis for the current version of MARS. The second phase of information processing focused on updating the MARS descriptive system (van der Heijde, 1994b). To incorporate new ground-water research developments and advances in software environments and to make the database more useful, the existing descriptive system was revised and expanded. The new descriptive system was implemented in version 4.1 of MARS. A summary of the descriptive terms used in MARS version 4.1 is given in Table 1. In converting the contents of the earlier version of the database to this new version, many of the existing records were edited, corrected, and expanded. In the third and final phase of data collection and evaluation, more than 300 new descriptions were added to the database, resulting in a total of 823 records at the end of September 1994.

Major Software Categories in MARS

There are thirty-seven (37) major software categories classified in MARS version 4.1 (van der Heijde, 1994b). These categories range from flow and transport (*e.g.*, saturated flow, unsaturated flow, solute transport, heat transport, virus transport), to test analysis (*e.g.*, aquifer test analysis, tracer test analysis), to parameter identification (*e.g.*, inverse model, dual porosity medium), and finally to lumped parameter approaches (*e.g.*, water budget, heat budget, chemical mass balance). The entire list of categories is given in Table 2 with the name of the category and a brief description of the type of software stored under that name.

Preparation of Information Tables

The tables presented in Appendices A-E in the full report were prepared using specially designed database reports in the MARS application using R:Base Version 4.5 Plus ™ for MS-DOS. The specific search and sort criteria used in the preparation of the appendices is detailed in the full report.

The tables which occur in the various appendices of the full report are listed below:

Table 1. Summary of descriptive terms used in MARS version 4.1.

General Information

- IGWMC software identification number (IGWMC Key)
- Software name, current version and release date
- Software authors
- Model category/type
- Development objective
- Abstract (short description of major software characteristics)
- Computer hardware / software requirements
- IGWMC evaluation of documentation and code testing
- Code input processing capabilities
- Code output processing capabilities
- Terms of code availability
- Availability of model support
- Name and address of code distributor
- Name and address of code custodian organization
- Name and address of code development organization

Details

- Problem dimensionality capabilities
- Hydrogeologic and/or soil layering structure
- Flow, solute transport, heat transport and matrix deformation processes addressed
- Flow system characteristics
- Soil/rock material type
- Hydrogeochemical processes included
- Boundary conditions supported
- Numerical grid characteristics
- Mathematical solution techniques (formulation, solvers, inverse approaches, optimization)
- Input requirements
- Output capabilities
- Pertinent literature references

Table A-1. A cross-reference table for ground-water modeling software alphabetized by program name, giving model name, authors, IGWMC key, and the Appendix C page number of the detailed software descriptions (531 records).

Table A-2. The same as Table A-1, except the ordering is by IGWMC key, rather than by model name.

Table B-1.1. Single-phase flow in the saturated zone—analytical models (43 records).

Table B-1.2. Single-phase flow in the saturated zone—numerical models (194 records).

Table B-2. Single-phase flow in the unsaturated zone—(109 records).

Table B-3. Pathline and capture zone analysis (44 records).

Table B-4.1. Solute transport in the saturated zone—analytical models (47 records).

Table B-4.2. Solute transport in the saturated zone—numerical models (93 records).

Table B-5. Solute transport in the unsaturated zone (59 records).

Table B-6. Heat transport (50 records).

Table B-7. Saltwater intrusion (20 records).

Table B-8. Multiphase flow and transport (14 records).

Table B-9. Vapor transport (21 records).

Table B-10. Virus transport (2 records).

Table B-11. Fluid flow and rock deformation (21 records).

Table B-12.1. Parameter estimation—aquifer/slug test analysis (33 records).

Table B-12.2. Parameter estimation—numerical saturated zone flow (7 records).

Table B-12.3. Parameter estimation—unsaturated zone flow (6 records).

Table B-12.4. Parameter estimation—transport and tracer test analysis (5 records).

Table B-13. Geochemical models (31 records).

Table B-14. Optimization/management models (9 records).

Table B-15. Simulation models for fractured rock (33 records).

Table B-16. Geostatistical analysis and stochastic simulation (22 records).

Table B-17. Ground-water related exposure/risk assessment (7 records).

Table C. Detailed software descriptions sorted by IGWMC key (531 records).

Table D. Software references sorted by IGWMC key--proceedings of conferences, peer-reviewed references, government reports, user's manuals, etc. (1145 records).

Table E-1. Cross-reference table for software distributors (organization/name, address, telephone and fax numbers)—sorted by IGWMC key (37 records).

Table E-2. Same as Table E-1 sorted by distributor identification number.

Table 2. Major software categories as classified in MARS version 4.1

Category	*Term*	*Description*
1	saturated flow	ground-water flow in the saturated zone; including pathline, streamline, and capture zone models based on flow equations
2	unsaturated flow	flow of water in the unsaturated zone; single phase or in conjunction with air flow
3	vapor flow/transport	movement of vapor in soils and chemical interaction between vapor phase and liquid and/or solid phase
4	solute transport	movement and (bio-)chemical transformation of water dissolved chemicals and their chemical interaction with the soil or rock matrix
5	heat transport	transport of heat in (partially) saturated rock or soil
6	matrix deformation	deformation of soil or aquifer rock due to removal or injection of water or changes in overburden
7	geochemical	chemical reactions in the fluid phase and between the fluid phase and the solid phase
8	optimization (optimization)	flow or transport models which includes mathematical optimization to develop a 'best' management strategy
9	ground-water/surface water hydraulics	interaction between ground water and surface water described in terms of fluid mass exchanges; hydraulics of both ground water and surface water are described
10	parameter ID unsaturated flow	calculation of the parameters of the soil hydraulic functions from laboratory measurements
11	inverse model	numerical models for distributed flow and/or transport parameter identification in the saturated zone
12	aquifer test analysis	analytical or numerical models for evaluation of aquifer flow parameters from pumping tests
13	tracer test analysis	analytical or numerical models for evaluation of aquifer transport parameters from tracer tests
14	water/steam flow	heat transport models in which both the liquid and steam phases are described and phase changes supported
15	fresh/salt water flow	sharp interface approach with either fresh water flow only, or flow in both the fresh- and salt-water zone
16	multiphase flow	flow of water, NAPL and/or air/vapor
17	watershed runoff	watershed surface-, stream-, and ground-water runoff
18	surface water runoff	stream runoff routing
19	sediment transport	surface sediment transport
20	virus transport	transport of viruses
21	biochemical transformation	hydrochemical or solute transport models which include specific biochemical reactions and population growth/die-off equations
22	pre-/postprocessing	model input preparation and output reformatting or display
23	stochastic simulation	including Monte Carlo analysis
24	geostatistics	kriging
25	multimedia exposure/risk analysis	exposure assessment/risk analysis models for ground-water, surface water and atmospheric pathways
26	expert system	ground-water oriented advisory system
27	database	ground-water application-oriented database
28	ranking/screening	classification; no simulation
29	fracture network	no primary porosity, connected fractures only; discrete network of fractures connected at network nodes
30	porous medium	default medium type; primary porosity only
31	dual porosity medium	fractured porous medium with porous blocks intersected by connected or non-connected fractures; mass exchange between fractures and porous blocks
32	porous medium,fractures	porous medium with individual fractures
33	karst	models specifically designed for karst systems (pipe flow, non-Darcian flow, etc.)
34	water budget	lumped parameter approach for ground-water flow
35	heat budget	lumped parameter approach for heat flow
36	chemical mass balance	lumped parameter approach for solute transport
37	water level conversion	converting water level observations to velocities using Darcy's law

Conclusions

The full report provides a catalogue of over 500 computer programs for analyzing ground-water problems. Many of the programs include simulation capabilities allowing the user to perform quantitative analyses of fluid flow, vapor transport and contaminant migration problems in the saturated and/or unsaturated zone. The simulation models considered range from simple mass balance calculations to sophisticated, multi-dimensional numerical simulators. Many of the more recent computer programs include sophisticated user-interfaces and graphic output capabilities. Increasingly, ground-water modeling software includes peripheral programs for geostatistical analysis and data management, or separate programs are being developed for this purpose. Linkages with general purpose commercial software (*e.g.,* spreadsheet, CAD, GIS, contouring, and line graphing software) are becoming common. Sometimes, ground-water simulation software is embedded in a risk assessment framework or an expert system shell.

The full report does not pretend to be a complete listing of ground-water modeling related software. Almost every week, the International Ground Water Modeling Center is informed of new computer codes addressing some aspect of fluid flow and contaminant behavior in the subsurface, as well as approaches to mitigation and prevention of pollution problems. Moreover, many codes have been developed primarily for research purposes and are not readily accessible. Also, there are many simple models based on mass balance evaluation or analytical solution of highly simplified systems not presented in this catalogue. An effort has been made to select those *simple* models which are either known for their use in a regulatory or enforcement mode, or which are considered representative for a certain type of models.

In compiling the information for the catalogue, some relevant issues have arisen. In many cases, ground-water modeling documentation is insufficient to determine the actual implementation of boundary conditions in the code, or the required detail in discretization in the spatial and temporal domains. Running a model code, using test problems different than the example problems provided in the documentation, might reveal specific model characteristics concerning accuracy, stability, data preparation, or execution problems. This exercise will also provide insights to *tricks* to handle these types of problems. It should be noted that most ground-water modeling software address only a limited number of conditions encountered in the field.

The full report provides readers an overview of available ground-water modeling programs and related software. It serves as a first screening tool for selection of software for a particular application. Initially, when used for software selection, a few programs should be identified for further evaluation. Such evaluation should be based on analysis of software documentation, and in some cases, test execution of the demonstration versions or fully executable versions of the modeling programs. To provide guidance to this process, pertinent documentation references for the software are listed in Appendix D of the report.

References

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Paul K.M. van der Heijde is with the International Ground Water Modeling Center, Institute for Ground-Water Research and Education, Colorado School of Mines, Golden, CO 80401-1887.

Joseph R. Williams *is the EPA Project Officer (see below).*
The complete report, entitled "Compiliation of Saturated and Unsaturated Zone Modeling Software, Update of EPA/600/R-93/118 and EPA/600/R-94/028," (Order No. PB) Cost: , subject to change) will be available only from

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:
Subsurface Protection and Remediation Division
National Risk Management Research Laboratory
U.S. Environmental Protection Agency
Ada, OK 74820