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Project Summary

Quality Assurance and Quality Control in the Development and Application of Ground-water Models

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This report describes quality assurance and code testing in ground-water modeling. The quality assurance procedures presented cover both development and application of ground-water modeling codes. An important part of quality assurance is code testing and performance evaluation. The section on code testing and performance evaluation discusses past efforts to test ground-water simulation codes and document their performance and presents the three-level testing procedure developed by the International Ground Water Modeling Center and the Center's approach to developing benchmarks for the first two test levels.

This Project Summary was developed by EPA's Robert S. Kerr Environmental 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

Ground-water modeling has become an important methodology in support of the planning and decision-making processes involved in ground-water management. The effective application of computer simulation codes in modeling field problems is a qualitative procedure, a combination of science and art. A successful model application requires a combination of knowledge of scientific principles, mathematical methods, and site characterization paired with expert insight in the modeling process, often to be provided within the framework of a multi-disciplinary team effort. As participants at the workshop on "Modeling for Water Management" organized by the European Institute for Water (Como, Italy, May 21-22,1987) formulated: "Modeling imposes discipline by forcing all concerned to be explicit on goals, criteria, constraints, relevant processes, and parameter values."

Ground-water models provide an analytical framework for obtaining an understanding of the mechanisms and controls of ground-water systems and the processes that influence their quality, especially those caused by human intervention in such systems. For managers of water resources, models may provide essential support for planning and screening of alternative policies, regulations, and engineering designs affecting groundwater. This is particularly evident with respect to ground-water resources development, ground-water protection, and aquifer restoration.

In discussing ground-water modeling, distinction should be made between model development and model application. Model development consists of three components: (I) research aimed at obtaining a quantitative understanding of the studied ground-water system; (2) software development; and (3) model testing and evaluation. Often, model development, and particularly code development, is driven by immediate and long-term needs of ground-water resources management. Model application is part of a larger set of activities aimed at solving site- or problem-specific issues and includes such activities as data collection, interpretation and storage, system conceptualization and model design, formulation of alternative problem solving scenarios and engineering designs, and post-simulation analysis.

Although a consensus may exist as to what ground-water modeling entails, the definition of a "model" *per se* is somewhat nebulous. In hydrogeology, the term "ground-water model" has become synonymous with conceptual ground-water models, mathematical ground-water models (including analytical and numerical models), computer models, and simulation models. Furthermore, the term "ground-water model" may apply either to a computer code without site-specific data or to the representation of a site-specific system using such a generic code, together with pertinent data.

In the full report a ground-water model is defined as a non-unique, simplified, mathematical description of the subsurface component of a local or regional hydrologic system, coded in a computer programming language, together with a quantification of the simulated system in the form of boundary conditions, system and process parameters, and system stresses. The generalized computer code usable for different site- or problem-specific simulations is referred to as a (computer) simulation code or a generic simulation model. A ground-water modeling study is defined as the development and use of a ground-water model (i.e., code and data) to solve specific ground-water management problems. Sometimes, such a ground-water model is the result of the application of one or more simulation codes to a generalized ground-water management problem; e.g., in support of promulgating government-mandated regulations. Generalizing such a management problem may be based on the use of concepts and data describing an "average" or "hypothetical" site representing targeted sites.

Sometimes a model is described in terms of the mathematical solution technique employed. Most commonly used terms are "analytical model," "semi-analytical model," and "numerical model." An analytical model is a model in which the solution of the mathematical problem (governing equation and boundary conditions) results in a closed-form or analytical expression for the state variable, continuous in the space and time domains. In a numerical model a solution for the mathematical problem is found, discrete in both the space and time domains, by using numerical approximations of the governing partial differential equation(s). In a semianalytical model complex analytical solutions are approximated by numerical techniques, resulting in a discrete solution in either the space or time domain.

Developing efficient and reliable software and applying such tools in ground-water management requires a number of steps, each of which should be taken conscientiously and reviewed carefully. Taking a systematic, well defined and controlled approach to all steps of the model development and application process is essential for its successful utilization in management. Quality Assurance (QA) provides the mechanisms and framework to ensure that decisions are based on the best available data and (modeling-based) analyses.

Sections in the full report provide background information on quality assurance and define the role of QA in ground-water modeling. They present a functional and practical quality-assurance methodology, written from the perspective of the model user and the decision-maker in need of technical information on which to base decisions. An important part of quality assurance is code testing and performance evaluation. The section on code testing and performance evaluation presents the three-level testing procedure developed by the International Ground Water Modeling Center, the development of test problems and related benchmarks for the first two test levels, and a discussion of the implementation of the testing procedure.

Quality Assurance in Ground-water Modeling

Quality assurance in ground-water modeling is the procedural and operational framework put in place by the organization managing the modeling study, to assure technically and scientifically adequate execution of all project tasks included in the study, and to assure that all modeling-based analysis is verifiable and defensible. QA in ground-water modeling is crucial to both model development and model use and should be an integral part of project planning and be applied to all phases of the modeling process.

The two major elements of quality assurance are quality control (QC) and quality assessment. Quality control refers to the procedures that ensure the quality of the final product. These procedures include the use of appropriate methodology in developing and applying computer simulation codes, adequate verification and validation procedures, and proper usage of the selected methods and codes. To monitor the quality control procedures and to evaluate the quality of the studies, quality assessment is applied. Each project should have a quality assurance plan (QA plan), listing the measures planned to achieve the project's quality objectives.

"Quality assurance" is a term used in many different disciplines and environments. Its meaning and implementation differs from field to field. For example, there is a significant difference between QA in software engineering, software quality assurance (SQA), and QA in industrial production. Also, there are significant differences between data QA and software QA procedures.

Literally, quality assurance assures the quality of the product (code, model) or activity of concern (modeling). A more workable description is that QA (in modeling) guarantees that the quality of the model-based analysis and advice (to decision-makers) satisfies quantitative quality criteria or measures. As the principal idea behind QA is accountability, and the main mechanism is maintaining records (hard copy and electronic files, reports) of all activities and results, a more proper term might be quality documentation.

Taken in a broad sense, QA provides a methodological and administrative framework to do the best we can within the limitations of our current understanding of nature and available technology.

That QA always assures acceptable quality of a code development project or a modeling study is an idle hope. However, adequate QA can provide safeguards against faulty codes or improper modeling. Regulators and decision-makers should understand that there is no way to guarantee that modeling-based advice is entirely correct, nor that the simulation code used (or any scientific model or theory, for that matter) can ever be proven, verified or validated in the strictest sense of these terms. Rather, a model can only be invalidated by disagreement of its predictions with independently derived observations regarding real systems.

It should be noted that a major role of QA/QC is to provide communication between the modeler and his/her peers, and between modeler and decision-maker, giving the latter a sense of the accuracy, uncertainty, and reliability of the modeler's advice. Therefore, QA should not apply to the work of junior modelers only, but should also be adhered to by expert modelers.

There are various cautions to be made. QA should never become so stifling that experienced modelers are discouraged to take new avenues not previously explored, or that an inappropriately large part of the budget of a project is consumed by responding to bureaucratic requirements.

When QA regulations become bureaucratic red tape, the time and cost of QA may take away precious resources from the data collection and problem analysis activities. Furthermore, the risk is present that QA deteriorates and becomes only a checklist installing false confidence in modeling results.

Code Testing and Evaluation Procedures

The usefulness of predictive simulations based on ground-water models is often limited by our inability to indicate and quantify the reliability of such model results. Researchers have developed various techniques to assess confidence levels for model predictions, so that water resources managers can account for uncertainties in the decision-making process. For example, several investigators present a methodology based on the application of decision analysis to engineering design in a hydrogeological environment. The methodology involves the coupling of a decision model based on a risk-cost-benefit objective function, a simulation model for ground-water flow and contaminant transport, and an uncertainty model that encompasses both geological uncertainty and parameter uncertainty.

One area of concern is the credibility of the simulation codes used and the generic models they represent. As discussed in the full report, an important aspect of the credibility of a simulation code is its reliability. The reliability of codes is established by applying a comprehensive, systematic review and testing procedure. The quality assurance aspects of such a procedure have been discussed in Section 2.2 of the full report. Another section presents a systematic code verification and performance testing protocol, based on the use of analytical solutions and synthetic data sets as benchmarks. Although the full report provides some example test problems, it does not contain actual benchmarks. A comprehensive set of benchmarks for two- and three-dimensional ground-water flow and transport models will be presented in a follow-up report.

Conclusions

There is an urgent need for comprehensive, systematic testing of all types of ground-water models and for the establishment of a verification and validation protocol. Ground-water management decisions should be based on the use of technically and scientifically sound methods of data collection, information processing, and interpretation. Because few experimental investigations have tested multidimensional theories, conceptualization, and associated computer codes, it is extremely important to conduct further research aimed at developing and executing verification and validation studies for prominent ground-water models. It may be argued that from a ground-water management point of view further efforts should be directed towards model testing studies rather than toward the development of more complex models.

In recent years, the International Ground Water Modeling Center has developed a testing procedure and methodology for model evaluation as part of its efforts to implement a comprehensive quality assurance program. The current project attempts to systematically analyze the scientific considerations and collect the technical elements for implementation of such a methodology. The next step is the application of this comprehensive methodology to actual computer codes.

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The complete report, entitled "Quality Assurance and Quality Control in the Development and Application of Ground-water Models," (Order No. PB93-178226; Cost: $19.50; subject to change) will be available only from

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