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Quality Assurance in Computer Simulations of Groundwater Contamination

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ABSTRACT

In the development of policies and regulations for groundwater protection, in permitting, and in planning monitoring and remedial actions, the role of mathematical models is growing rapidly. Because water-resource management decisions should be based on technically and scientifically sound methods, quality assurance (QA) needs to be applied to groundwater modeling, both in model development and field studies, and should also play an important part in model selection.

Important aspects of QA in groundwater model development are peer review, and verification and validation of the computer code and its underlying theoretical principles. This paper discusses the role of review and testing as part of an overall QA approach, and addresses QA in model selection and field application.

Key Words: groundwater, mathematical models, quality assurance, model validation, pollution, model selection

INTRODUCTION

The science of groundwater flow and contaminant transport is not yet an exact field of knowledge. Although the physical processes involved obey known mathematical and physical principles, exact aquifer and contaminant characteristics are hard to obtain and often make even plume definition a difficult task. However, where these characteristics have been reasonably established, groundwater models may provide a viable, if not the only, method to predict contaminant transport, to locate areas of potential environmental risk, and to assess possible remediation/corrective actions [1].

Mathematical models are used to help organize the essential details of complex groundwater management problems so that reliable solutions are obtained. Applications include a wide range of technical, economic, and sociopolitical aspects of groundwater supply and protection [2, 3, 4, 5].

A groundwater protection policy based on monitoring is by its very nature always reactive, not preventive; however, model-based policies and regulations can be both preventive and reactive. Because adequate on-site monitoring is not always feasible due to costs, available manpower, or site accessibility, models can provide a viable and effective alternative. An optimal approach to the management of groundwater resources includes the integrated use of modeling and monitoring strategies.

The role of groundwater-flow and contaminant-transport models in the development of policies and regulations, in permitting, and in planning of monitoring and remedial action, is continuing to grow. Some of the principal areas where mathematical models can now be used to assist in the management of groundwater protection programs are [6]:

- development of regulations and policies
- planning and design of corrective actions and waste storage facilities
- problem conceptualization and analysis
- development of guidance documents
- design and evaluation of monitoring and data collection strategies
- enforcement

Specifically, groundwater modeling plays or can play a role in:

- determining or evaluating the need for regulation of specific waste disposal, agricultural, and industrial practices
- analyzing policy impacts such as evaluating the consequences of setting regulatory standards and banning rules, and of delisting actions
- assessing exposure, hazard, damage, and health risks
- evaluating reliability, technical feasibility and effectiveness, cost, operation and maintenance, and other aspects of waste-disposal facility designs and of alternative remedial actions
- providing guidance in siting of new facilities and in permit issuance and petitioning
- detecting pollutant sources
- developing aquifer or well-head protection zones
- assessing liabilities such as post-closure liability for disposal sites

These activities can be broadly categorized as either site-specific or generic modeling efforts, and these categories can be further subdivided into point-source or non-point-source problems. The success of these modeling efforts depends on the accuracy and efficiency with which the natural processes controlling the behavior of groundwater, and the chemical and biological species it transports, are simulated. The accuracy and efficiency of the simulations, in turn, depend heavily on the applicability of the assumptions and simplifications adopted in the model(s), on the availability of reliable data, and on subjective judgments made by the modeler and management.

If litigation is involved, the model code itself and its theoretical foundation may become contested. There-

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fore, adequate guidelines should be developed for selection of simulation codes to be used under such circumstances. Such guidelines should cover code review, validation, and documentation and should be widely accepted.

It is of the highest importance that water resource management decisions be based on the use of technically and scientifically sound data collection, information processing, and interpretation methods. Quality Assurance (QA) provides the mechanisms to ensure that decisions are based on the best available data and analyses. This paper discusses QA guidelines applicable to groundwater modeling and the role of QA in the model selection process.

QUALITY ASSURANCE IN GROUNDWATER MODELING

Quality assurance in groundwater 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 [7]. QA in groundwater modeling should be applied to both model development and model application and should be an integral part of all projects. 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, adequate validation, and proper usage.

To monitor the quality control procedures and to evaluate the quality of the products of field studies, quality assessment is applied. It consists of two elements: auditing and technical review. Audits are procedures designed to assess the degree of compliance with QA requirements, commensurate with the level of QA prescribed for the project. Compliance is measured in terms of traceability of records, accountability (approvals from responsible staff), and fulfillment of commitments in the QA plan. Technical review consists of independent evaluation of the technical and scientific basis of a project and the usefulness of its results.

QA is the responsibility of both the project team (quality control and internal evaluation) and the contracting or supervising organization (quality assessment). QA should not drive or manage the direction of a project nor is QA intended to be an after-the-fact filing of technical data.

Various phases of quality assessment exist for both model development and application. First, review and testing is performed by the author, and sometimes by other employees not involved in the project, or by invited experts from outside the organization. Also to be considered is the quality assessment by the organization for which the project has been carried out. Again, three levels can be distinguished: project or product review or testing by the project officer or project monitor, by technical experts within the funding or controlling organization, and by an external peer review group.

Decisions by natural resources and environmental managers rest on the quality of environmental data and data analysis; therefore, program managers in regulatory agencies should be responsible for: (1) specifying the quality of the data required from environmentally related measurements and for the level of problem-solving data analysis; and (2) providing sufficient resources to assure an adequate level of QA.

QA procedures should be contained in a QA plan to be developed for each modeling study. The plan lists the measures required to achieve prescribed quality objectives. Major elements of such a QA plan are: (1) formulation of QA objectives and required quality level in terms of validity, uncertainty, accuracy, completeness, and comparability; (2) development of operational procedures and standards for performing adequate modeling studies; (3) establishing a paper trail for QA activities in order to document that standards of quality have been maintained; and (4) internal and external auditing and review procedures. The QA plan should also specify individual responsibilities for achieving these goals.

Model Development

Ideally, QA should be applied to all codes currently in use and yet-to-be-developed codes. Relevant QA procedures include such aspects as the verification of the mathematical framework, field validation, benchmarking, and code comparison. A detailed discussion of model testing and review is described in the second part of this paper.

QA for code development and maintenance should include complete record-keeping of the model development, of modifications made in the code, and of the code-validation process. The paper trail for QA in model development consists of reports and files on the development of the model. The reports should include a description of:

- assumptions
- parameter values and sources
- boundary and initial conditions
- nature of grid and grid design justification
- changes and verification of changes made in code
- actual input used
- output of model runs and interpretation
- validation (or at least calibration) of model

In addition, depending on the level of QA required, the following files may be retained (in hard-copy and, at higher levels, in digital form):

- version of source code used
- verification input and output
- validation input and output
- application input and output

If any modifications are made to the model coding for a specific problem, the code should be tested again; all QA procedures for model development should again be applied, including accurate record keeping and reporting. All new input and output files should be saved for inspection and possible reuse.

Model Application

QA in model application should address all facets of the model application process:

- correct and clear formulation of problems to be solved
- project description and objectives
- modeling approach to the project
- is modeling the best available approach and if so, is the selected model appropriate and cost-effective?
- conceptualization of system and processes, including hydrogeologic framework, boundary conditions, stresses, and controls
- explicit description of assumptions and simplifications
- data acquisition and interpretation
- model selection, or justification for choosing to develop a new model
- model preparation (parameter selection, data entry or reformatting, gridding)
- the validity of the parameter values used in the model application
- protocols for parameter estimation and model cali-

bration to provide guidance, especially for sensitive parameters
- level of information in computer output (variables and parameters displayed; formats; layout)
- identification of calibration goals and evaluation of how well they have been met
- sensitivity analysis
- postsimulation analysis (including verification of reasonability of results, interpretation of results, uncertainty analysis, and the use of manual or automatic data processing techniques, as for contouring)
- establishment of appropriate performance targets (e.g., 6-foot head error should be compared with a 20-foot head gradient or drawdown, not with the 250-foot aquifer thickness!); these targets should recognize the limits of the data
- presentation and documentation of results
- evaluation of how closely the modeling results answer the questions raised by management

A major problem in model use is model credibility. In the selection process special attention should be given to ensure the use of qualified models that have undergone adequate review and testing.

As is the case with model development QA, all data files, source codes, and executable versions of computer software used in the modeling study should be retained for auditing or postproject re-use.

MODEL REVIEW AND TESTING

Before a groundwater model is used as a planning and decision-making tool, its credentials must be established, independently of its developers, through systematic testing and evaluation of the model's characteristics. Code testing is generally considered to encompass verification and validation of the model [8]. To evaluate groundwater models in a systematic and consistent manner, the International Ground Water Modeling Center (IGWMC) has developed a model review, verification, and validation procedure [5]. Generally, the review process is qualitative in nature, while code testing results can be evaluated by quantitative performance standards.

Model Review

A complete review procedure comprises examination of model concepts, governing equations, and algorithms chosen, as well as evaluation of documentation and general ease-of-use, and examination of the computer coding [5, 9]. If the model has been verified or validated by the author, the review procedure should include evaluation of this process.

To facilitate thorough review of the model, detailed documentation of the model and its developmental history is required. In addition, to ensure independent evaluation of the performed verification and validation, the computer code should be available or at least accessible for implementation on the reviewer's computer facilities, together with a file containing the original test data used in the code's verification and validation.

Review should be performed by experienced modelers knowledgeable in theoretical aspects of groundwater modeling. Because review is rather subjective in nature, selection of the reviewers is a sensitive and critical process.

Model Examination

Model examination determines whether anything fundamental was omitted in the initial conceptualization of the model. Such a procedure determines whether the concepts of a model adequately represent the nature of the system under study, and identifies the processes and actions pertinent to the model's intended use. The examination also determines whether the equations representing the various processes are valid within the range of the model's applicability, whether these equations conform mathematically to the intended range of the model's use, and whether the selected solution approach is the most appropriate. Finally, model examination determines the appropriateness of the selected initial and boundary conditions and establishes the applicability range of the model.

For complex models, detailed examination of the implemented algorithms is required to determine whether appropriate numerical schemes, in the form of a computer code, have been adopted to represent the model [10]. This step should disclose any inherent numerical problems such as non-uniqueness of the numerical solution, inadequate definition of numerical parameters, incorrect or nonoptimal values used for these parameters, numerical dispersion, numerical instability such as oscillations or divergent solution, and problems regarding conservation of mass.

In addition, the specific rules for proper application of the model should be analyzed from the perspective of its intended use. These rules include data assignment according to node-centered or block-centered grid structure for finite-difference methods; size and shape of elements in integrated finite-difference and finite-element methods; grid size variations; treatment of singularities such as wells; approach to vertical averaging in two-dimensional horizontal models or layered three-dimensional models; inclusion of partial solutions in analytical element methods; and treatment of boundary conditions. Consideration is also given to the ease with which the mathematical equations, the solution procedures, and the final results can be physically interpreted.

Evaluation of Model Documentation

Model documentation is evaluated through visual inspection, comparison with existing documentation standards and guidelines, and through its use as a guide in preparing for and performing verification and validation runs.

Good documentation includes a complete treatment of the equations on which the model is based, of the underlying assumptions, of the boundary conditions that can be incorporated in the model, of the method used to solve the equations, and of the limiting conditions resulting from the chosen method. The documentation must also include a user's manual containing instructions for operating the code and preparing data files, example problems complete with input and output, programmer's instructions, computer operator's instructions, and a report of the initial code verification.

Evaluating Ease of Use

The data files provided by the model developer are used to evaluate the operation of the code and the user's guide through a test-run process. In this stage special attention is given to the rules and restrictions ("tricks," e.g., to overcome restrictions in applicability) necessary to operate the code, and to the code's ease-of-use aspects [11].

Computer Code Inspection

Part of the model review process is the inspection of the computer code. In this inspection attention is given to the manner in which modern programming principles have been applied with respect to code structure, optimal use of the programming language, and internal documentation. This step helps reveal undetected programming or logic errors, hard to detect in verification runs.

MODEL VERIFICATION

The objective of the the verification process is twofold: (1) to check the accuracy of the computational algorithms used to solve the governing equations, and (2) to assure that the computer code is fully operational.

To check the code for correct coding of theoretical principles and for major programming errors ("bugs"), the code is run using problems for which an analytical solution exists. This stage is also used to evaluate the sensitivity of the code to grid design, to various dominant processes, and to a wide selection of parameter values [9, 12, 13, 14].

Although testing numerical computer codes by comparing results for simplified situations with those of analytical models does not guarantee a fully debugged code, a well-selected set of problems ensures that the code's main program and most of its subroutines, including all of the frequently called ones, are being used in the testing. In the three-level test procedure developed by the International Ground Water Modeling Center (IGWMC), this type of testing is referred to as level I [15].

Hypothetical problems are used to test special features that cannot be handled by simple close-form solutions, as in testing irregular boundary conditions and certain heterogeneous and anisotropic aquifer properties; this is the IGWMC level II testing.

For both level I and level II testing, sensitivity analysis is applied to further evaluate code characteristics.

MODEL VALIDATION

Model validation or field validation is defined as the comparison of model results with numerical data independently derived from laboratory experiments or observations of the environment [10]. Complete model validation requires testing over the full range of conditions for which the model is designed. Model development is an evolutionary process responding to new research results, developments in technology, and changes in user requirements. Model review and validation needs to follow this dynamic process and should be applied each time the model is modified.

The objective of model validation is to determine how well the model's theoretical foundation describes the actual system behavior in terms of the "degree of correlation" between model calculations and actual measured data for the cause-and-effect responses of the system. Obviously, a comparison with field data is required. Such a comparison may take either of two forms. One form, calibration, is sometimes considered the weaker form of validation insofar as it tests the ability of the code (and the model) to fit the field data, with adjustments of the physical parameters [13]. Some researchers prefer to classify calibration as a form of verification rather than a form of validation.

The other form of validation is that of prediction. This is a test of the model's ability to fit the field data with no adjustments of the physical parameters. In principle, this is the correct approach to validation. However, unavailability and inaccuracy of field data often prevent such a rigid approach. Typically, a part of the field data is designated as calibration data, and a calibrated site-model is obtained through reasonable adjustment of parameter values. Another part of the field data is designated as validation data; the calibrated site model is used in a predictive mode to simulate similar data for comparison. The quality of such a test is therefore determined by the extent to which the site model is "stressed beyond" the calibration data on which it is based [13]. In the IGWMC testing procedure, this approach is referred to as level III testing.

For many types of groundwater models, a complete set of test problems and adequate data sets for the described testing procedure is not yet available. Therefore, testing of such models is generally limited to extended verification, using existing analytical solutions, and to code intercomparison.

Whether a model is valid for a particular application can be assessed by performance criteria, sometimes called validation or acceptance criteria. If various uses in planning and decision making are foreseen, different performance criteria might be defined. The user should then carefully check the validity of the model for the intended use.

Three levels of validity can be distinguished [10]:

(1) Statistical Validity: using statistical measures to check agreement between two different distributions, the calculated one and the measured one; validity is established by using an appropriate performance or validity criterion.

(2) Deviative Validity: if not enough data are available for statistical validation, a deviation coefficient D can be established, e.g.,

$$D = [(x-y)/x]100\%$$

where x = predicted value and y = measured value. The deviation coefficient might be expressed as a summation of relative deviations. If ED is a deviative validity criterion supplied by subjective judgment, a model can considered to be valid if $D < ED$.

(3) Qualitative Validity: using a qualitative scale for validity levels representing subjective judgment: e.g., excellent, good, fair, poor, unacceptable. Qualitative validity is often established through visual inspection of graphic representations of calculated and measured data [16].

The aforementioned tests apply to single variables and determine local-or-single variable validity; if more than one variable is present in the model, the model should also be checked for global validity and for validity consistency [10]. For a model with several variables to be globally valid, all the calculated outputs should pass validity tests. Validity consistency refers to the variation of validity among calculations having different input or comparison data sets. A model might be judged valid under one data set but not under another, even within the range of conditions for which the model has been designed or is supposedly applicable. Validity consistency can be evaluated periodically when models have seen repeated use.

Often, the data used for field validation are not collected directly from the field but are processed in an earlier study. Therefore, they are subject to inaccuracies, loss of information, interpretive bias, loss of precision, and transmission and processing errors, resulting in a general degradation of the data.

As noted earlier, for many types of groundwater models no field data sets are available to execute a complete validation. One approach sometimes taken is that of code intercomparison, where a newly developed model is compared with existing models designed to solve the same type of problems as the new model. If the simulation results from the new code do not deviate significantly from those obtained with the existing code, a relative or comparative validity is established. It is obvious that as soon as adequate data sets become available, all the involved models should be validated with those data.

Further development of databases for field validation of solute transport models is necessary. This is also the case for many other types of groundwater models. These research databases should represent a wide variety of hydrogeological situations and should reflect the various types of flow, transport, and deformation mechanisms present in the field. The databases should also contain extensive information on hydrogeological, soil, geochemical, and climatological characteristics. With the development of such databases and the adoption of standard model-testing and validation procedures, the reliability of models used in field applications can be improved considerably.

Validation Scenarios

Often, various approaches to field validation of a model are viable. Therefore, the validation process should start with defining validation scenarios. Planning and conducting field validation should include the following steps [17]:

(1) Define data needs for validation and select an available data set or arrange for a site to study.

(2) Assess the data quality in terms of accuracy (measurement errors), precision, and completeness.

(3) Define model performance or acceptance criteria.

(4) Develop strategy for sensitivity analysis.

(5) Perform validation runs and compare model performance with established acceptance criteria.

Sensitivity Analysis

An important characteristic of a model is its sensitivity to variations or uncertainty in input parameters. Sensitivity analysis defines quantitatively or semiquantitatively the dependence of a selected model performance assessment measure (or an intermediate variable) on a specific parameter or set of parameters [18]. Model sensitivity can be expressed as the relative rate of change of selected output caused by a unit change in the input. If the change in the input causes a large change in the output, the model is sensitive to that input. Sensitivity analysis is used to identify those parameters most influential in determining the accuracy and precision of model predictions. This information is of importance to the user, as he must establish required accuracy and precision in the model application as a function of data quantity and quality [17]. In this context the use of a sensitivity index as described by Hoffman and Gardner [19] is of interest. It should be noted that if models are coupled, as in multimedia transport of contaminants, the propagation of errors and the increase in uncertainty through the subsequent simulations must be analyzed as part of the sensitivity analysis.

MODEL SELECTION

Using models to analyze alternative solutions to groundwater problems requires a number of steps, each of which should be taken conscientiously and reviewed carefully. After the decision to use an existing model has been made, the selection process is initiated. As model credibility is a major problem in model use, special attention should be given in the selection process to ensure the use of qualified models that have undergone adequate review and testing. Selecting an appropriate model is crucial to the success of a modeling project.

Model selection is the process of matching a detailed description of the modeling needs with well-defined, quality-assured characteristics of existing models, while taking into account the objectives of the study and the limitations in the personnel and material resources of the modeling team. In selecting an appropriate model, both the model requirements and the characteristics of existing models must be carefully analyzed. Major elements in evaluating modeling needs are: (1) formulation of the management problems to be solved and the level of analysis sought; (2) description of the system under study; and (3) analysis of the constraints in human and material resources available for the study. Model selection is partly quantitative and partly qualitative. Many subjective decisions must be made, often because there are insufficient data in the selection stage of the project to establish the importance of certain characteristics of the system to be modeled.

Definition of modeling needs is based on the management problem at hand, questions asked by planners and decision makers, and on the understanding of the physical system, including the pertinent processes, boundary conditions, and system stresses. The major criteria in selecting a model are: (1) that the model is suited for the intended use; (2) that the model is thoroughly tested and validated for the intended use; and (3) that the model code and documentation are complete and user-friendly.

Regardless of whether problem-solving performance standards are set, management-oriented criteria need to be developed for evaluating and accepting models. Such a set of scientific criteria should include:

- trade-offs between costs of running a model and accuracy
- profile of model user and definition of required user-friendliness
- accessibility in terms of effort, cost, and restrictions
- acceptable temporal and spatial scale and level of aggregation

If different problems must be solved, more than one model might be needed or a model might be used in more than one capacity. In such cases, the model requirements for each of the problems posed have to be clearly defined at the outset of the selection process. To a certain extent this is also true for modeling the same system in different stages of the project. Growing understanding of the system and data availability might lead to a need for a succession of models of increasing complexity. In such cases, flexibility of the model or model package might become an important selection criterion.

It should be realized that a perfect match rarely exists between desired characteristics and those of available models. Many of the selection criteria are subjective or weakly justified. If a match is hard to obtain, reassessment of these criteria and their relative weight in the selection process is necessary. Hence, model selection is very much an iterative process.

In standardizing model selection, three major approaches are employed in characterizing the validation of numerical models. In one, the model is tested according to established procedures; when accepted, the model is prescribed in federal or state regulations for use in cases covered by those regulations. This approach does not leave much flexibility for incorporating the advances of recent research and technological development. The second approach includes the establishment of a list of groundwater simulation codes as "standard" codes for various generic and site-specific management purposes. To be listed, a code should pass a widely accepted review and test procedure such as that described in a previous part of this paper. This approach is suggested in a recent evaluation of the role of modeling in the U.S. Environmental Protection Agency [6]. It should be noted that establishing "standard" models will not prevent discussion of the appropriateness of a selected model for analysis of a specific problem nor of its proper use in a particular decision-making process. In considering these two approaches, questions have been raised such as [6]:

- Are there legal liabilities for setting up certain models as acceptable? (For instance, if an enforcement agency certifies a model for use, can that agency no longer criticize an industry's use of that model?)
- Does certification squelch the development of new, better models?
- What balance should there be between using the newer, faster models and using mature models already subjected to peer review?

A third approach is to prescribe a review-and-test methodology in regulations of enforcement agencies, and require the model development team to show that the model code satisfies the requirements. This approach leaves room to update the codes as long as each version is adequately reviewed and tested. An example is the quality assurance program for models and computer codes of the U.S. Nuclear Regulatory Commission [20].

In any case, a general framework of nondiscriminatory criteria should be established [6]. These criteria should include:

- publication and peer review of the conceptual and mathematical frame-work
- full documentation and visibility of the assumptions
- testing of the code according to prescribed methods; this should include verification (checking the accuracy of the computational algorithms used to solve the governing equations), and validation (checking the ability of the theoretical foundation of the code to describe the actual system behavior)
- trade secrets (unique algorithms that are not described) should not be permitted if they might affect the outcome of the simulations; proprietary codes are already protected by the copyright law

Finally, as model selection is very closely related to system concep-tualization and problem solving, "expert systems" integrating system conceptualization and model selection on a problem-oriented basis promise to be valuable tools.

Further information on groundwater model selection is presented in [21, 22, 23, 24].

SUMMARY

During the 1970s a rapidly increasing awareness of the threat posed to groundwater resources by human-induced chemical and biological pollution has accelerated the development of sophisticated simulation models. These models are based on mathematical descriptions of the physical, chemical, and biological processes that take place in a complex hydrogeological environment. The extensive need for these models in assessing current and potential water quality problems has resulted in two groups of modelers: (1) model developers who are research-oriented and who generally apply models only for verification and validation purposes, and (2) model users who apply models routinely to actual generic or site-specific groundwater problems. The economic consequences of model predictions and the potential liabilities incurred by their use have brought quality guarantees and code credibility to the forefront as major issues in groundwater modeling. Hence, quality assurance (QA) needs to be defined for both model development and model application. There is a significant difference between these two: the first is designed to result in a reliable code, and the second to interpret correctly the simulation results. Both require stringent QA procedures to be established and enforced. As model credibility has become a major concern, model selection should focus on those codes that have undergone adequate review and testing. To further increase the applicability of the models, good documentation and user-friendliness of the computer coding involved should receive proper attention.

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