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Is Current Hydrogeologic Research Addressing Long-Term Predictions?

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Abstract

Hydrogeology is a field closely related to the needs of society. Many problems of current national and local interest require predictions of hydrogeological system behavior, and, in a number of important cases, the period of prediction is tens to hundreds of thousands of years. It is argued that the demand for such long-term hydrogeological predictions casts a new light on the future needs of hydrogeological research. Key scientific issues are no longer concerned only with simple processes or narrowly focused modeling or testing methods, but also with assessment of prediction uncertainties and confidence, couplings among multiple physico-chemical processes occurring simultaneously at a site, and the interplay between site characterization and predictive modeling. These considerations also have significant implications for hydrogeological education. With this view, it is asserted that hydrogeological directions and education need to be reexamined and possibly refocused to address specific needs for long-term predictions.

Introduction

In any research field, it is useful, and indeed healthy, to occasionally sit back and take a broad view of the field to identify key directions and outstanding issues for further research. In the hydrological sciences, a number of such overviews were conducted by the National Research Council (NRC) over the years (NRC 1991, 1998, 1999, 2001a, 2001b, 2002, 2004a, 2004b). NRC (2001a) outlined an agenda for water resources research in the 21st century and discusses the coordination of water resources agenda among state/federal governments, research institutions, and other interested parties. The report also listed 43 research issues of importance. In addition, NRC (2001b) presented high-priority research opportunities in earth sciences based on a series of symposia held in conjunction with Geological Society of America (GSA) and American Geological Union (AGU) meetings. Six key research areas were identified, ranging from integrative studies of the critical zone (defined as the near-surface environment of rock, soil, water, air, and living organisms), to geobiology, and to planetary science. This report (NRC, 2001b) gave also a useful discussion of balanced portfolios of investigator-driven disciplinary research, a problem-focused program of multidisciplinary research, and an equipment-oriented program for new instrumentation and facilities. In a subsequent report, NRC (2002) reported on a number of very interesting discussions at a workshop on predictability and limits to prediction in hydrologic systems, mainly in the context of the global water cycle and climatic change. NRC (2004a) focused on the interfaces between atmospheric, surface, and subsurface portions of the hydrologic system (with their different time and space scales), assessing the state-of-knowledge and identifying research needs concerning three general issues related to ground water fluxes. The most recent report, NRC (2004b), followed up on NRC (2001a) and examined current and historical patterns and magnitudes of investments in water resources research, and discussed improved coordination, prioritization, and implementation of research in water resources.

Specifically with regard to the field of hydrogeology, two thought-provoking papers have been published in *Ground Water* in the last three years. The first is a discussion by Schwartz and Ibaraki (2001), based on an analysis of citation statistics with reference to a typical industry life-cycle curve. Their conclusion is that the hydrogeological research field has come to a point close to the border between mature and aging, and that there is a need for new research ideas and for a new paradigm that would provide new opportunities. The approach of Schwartz and Ibaraki (2001) is unconventional, and it would be interesting to apply it to other scientific fields of similar histories for comparative evaluation. Such an exercise would help in understanding the validity of this approach. The second paper is a *Ground Water* Issue Paper by Miller and Gray (2002). They disagreed with the methodology and conclusions of Schwartz and Ibaraki (2001), and presented a detailed “bottom-up” discussion of the many exciting and challenging issues in hydrogeology. Their conclusion is that much fundamental and important work in hydrogeological research is yet to be done.

The present paper takes a different perspective from these two papers by starting with the need for hydrological inputs to major problems facing society today, many of which require long-term predictions of system behavior. Then, some general thoughts and specific recommendations for future hydrogeological research directions in this particular context are presented. In general, this paper agrees with the view and conclusions of Miller and Gray (2001)—that much work remains to be done. However, it also points out the need to go beyond a narrow definition of hydrogeological research. Specifically, we believe that, for long-term predictions, much research is needed on multiple couplings among physico-chemical-biological processes occurring simultaneously at a site, on the interplay between site characterization and predictive modeling, and on assessments of prediction uncertainties. Such research emphases correspond perhaps to the “change” or “new paradigms” suggested by Schwartz and Obaraki (2001).

In the next section, a brief historical perspective is provided, together with the current role of hydrogeology in several problems of national and local importance, as examples. Following this, three key scientific areas related to predictive hydrogeology are

discussed. Some remarks on hydrogeology education are then presented, after which a few general comments conclude the paper.

Historical Perspective and Current Role of Hydrogeology

Historically, hydrology has always been a research field intimately related to the needs of society at large. Surface water supply, such as that from rivers and lakes, has been recognized to be closely associated with the development of human society and civilization. Indeed, ensuring adequate water supply has been the main focus of modern hydrological research since its beginnings. Scientific issues associated with water quality and ground water resources have come to the forefront in the last 30 years. Now, hydrogeology (sometimes called ground water hydrology), defined as the study of water flow and quality in the subsurface, is a key element in solving many problems of national and local interest, such as the following:

- (a) Water resources and quality management. In many areas in the world, ground water is critically needed as part of the water supply, with much consideration given to how to optimize the “conjunctive use” of both ground and surface water. Associated with this issue is the evaluation of water quality, which varies spatially and with depth. Reaction kinetics between ground water and the rock matrix need to be accounted for as water from depths flows to shallower levels, and as ground water mixes with surface water. Further, at the surface, the interactions among rock, soil, water, air, and living organisms are also important research topics; for example, in the context of ecohydrology (Hunt and Wilcox, 2003).
- (b) Environmental contamination and management. In many locations, ground water has been contaminated through chemical spills or mishandling, excessive use of agricultural pesticides and fertilizers, and leakage of chemical storage tanks. Many of these contaminated sites represent long-term hazards that need to be contained or remediated.

- (c) Liquid and solid waste (including nuclear waste) disposal. Wastes are generated in many human activities, such as chemical manufacturing processes, mining operations, and nuclear power plants. Disposal methods include landfills, deep injection into the subsurface and underground repositories. Safety assessment of such methods involves the study of ground water flow and transport as a key element.
- (d) Global water cycle and climatic change. Recent attention to climatic change and the global water cycle includes consideration of hydrogeology, which is needed to account for a proper water balance in the global water cycle. Its role is significant given the long time frame of global climatic change.
- (e) Other problems requiring the study of hydrogeological conditions. These include geo-sequestration of CO₂ injected deep underground, geothermal reservoir development, and petroleum reservoir exploitation. For example, not only are petroleum reservoir dynamics similar to that of hydrogeological processes, but petroleum production also generates (in practice) substantial wastewater that is commonly re-injected into the subsurface. This activity has a significant impact on ground water flow systems.

Common to all the problems described above is the need for prediction of future hydrogeologic system behavior. Further, with a number of these problems, such as safety of liquid and solid waste isolation, the prediction period required is hundreds of thousands of years or more into the future. Important decisions at the national and local levels will be based on these extremely long-term predictions. Thus, there is a great need to conduct research that would provide the proper scientific foundation for these long-term predictions. This requires perhaps fundamentally new thinking—a paradigm shift for future research directions in hydrogeology.

We shall not attempt to review specific key research topics in hydrogeology related to these problems. These are discussed in detail elsewhere, such as in NRC reports (2001a,

2001b, 2002, 2004a) and in Miller and Gray (2002). We shall point out three broad areas as important examples, that deserve particular attention because of the need for long-term predictions. They are (a) couplings of physico-chemical processes occurring simultaneously at a site, (b) the interplay between site characterization and predictive modeling, and (c) quantitative assessment of uncertainties and confidence level.

Couplings of Physico-Chemical Processes at a Site

Often, problems of concern to society are site-specific, involving the effects of hydrogeological processes coupled with processes of other disciplines, such as chemistry and rock mechanics, which are all present at the site. So far, significant progress has been made on doubly coupled processes, such as hydrochemistry and thermomechanical and hydromechanical effects. However, triple or quadruple couplings involving heat, hydraulic, chemistry, rock mechanics, or even microbiology are also possible. Many of these couplings may become important when we consider predictions into the far future. For example, the so-called coupled THMC processes that couple thermal (T), hydrological (H), rock mechanical (M), and chemistry (C) effects are of great interest to the safety assessment of a nuclear waste geologic repository in fractured rock (Stephansson et al. 1996; Hudson et al. 2001). Thus, the underground excavation required to build a repository will cause the region around the repository to be mechanically modified, with a change in the local permeability to fluid flow. Also, heat release from decay of the nuclear waste induces thermal-mechanical effects in the rock, which will also cause closure of rock fractures and thus a decrease in fracture permeabilities. Both heat transfer and fluid flow would impact chemical reactions; in particular, the slow transient chemical changes.

Another example is coupled THC processes involved in the injection of chemical waste deep underground for disposal. The injected liquid has a different temperature from that of the injection zone, and chemical reactions of the injected liquid with *in situ* formation water and with the rock minerals may result in gas production, dissolution of rock

materials, or precipitation of solutes. These will change the size of the pores in the rock, their local saturation, and thus the rock's effective hydraulic conductivity. In cases where phase change (i.e., boiling and condensation) also occurs, the effect may be even more significant. Coupling hydrogeology and hydrochemistry with microbiology is another type of coupled processes that may occur in a number of problems. The main interest in our context is the change in hydraulic conductivity caused by microbiological activities in the ground water, and also the possibility of faster transport of contaminants in the subsurface owing to colloidal transport.

The coupled processes discussed above are just examples. Other examples include coupling of disciplines in ecohydrology and in surface waste management. Much research is still needed in this field.

Interplay between Site Characterization and Predictive Modeling

Many problems of national and local interest focus on questions such as whether the contamination at a particular site is contained, or whether the waste emplaced at a site (for example, 500 m below ground) is isolated from the biosphere for the next 10,000 years and more. These site-specific questions require site characterization methods to investigate the features and structure of the site, as well as ongoing (or expected future) physico-chemical processes at the site. It is recognized that a site can never be fully characterized in detail. The degree of characterization depends on the questions or model predictions of interest to the problem at hand. The relationship between site characterization and model prediction requires careful study, and should be put on a solid scientific basis, if possible.

To properly characterize a site, we cannot apply just one or two methods. We need a suite of methods not only to identify different characteristics, but also to confirm the results from one method by another, to build confidence in our knowledge of a site. The different methods include surface geologic and geophysical surveys, well logging and

monitoring, crosshole geophysical imaging and tomography, transient pressure testing, and tracer migration tests. All data can be put into a geologic information system (GIS) that allows easy visualization of the structures at the site.

After substantial data on the site have been obtained, we would construct a so-called conceptual model of the site, including the geological structure, property parameters, boundary conditions, and the types of physico-chemical processes occurring at the site. In addition, other “state” variables, such as pressure-head distribution and salinity distribution, are also determined. These variables may vary with time, because the site may not be in hydraulic equilibrium and is thus in a transient state. We need to verify the internal consistency of such a conceptual model, such that the distributions of state variables in the region are consistent with the boundary conditions and the geological structures.

After conceptual model or models are established, we need to consider carefully the scenarios for evolution of conditions thousands of years into the future. These will form the external (boundary) conditions for predictive modeling. Considerable effort has been made in this direction to assess scenario development methods and practices (NEA, 2001), and to survey potential future events and estimate their probabilities (see, for example, NEA, 2003). These probabilities are then used in a Monte Carlo or probabilistic approach to predict future system behavior and its uncertainties.

When building the conceptual model, uncertainties in data and interpretations need to be evaluated and tracked. Many times, since data are incomplete, alternative conceptual models could well satisfy all available data. Methodologies to deal with multiple alternative models and their relationship with model predictions need to be developed.

Also, to study hydrogeology at the site level, we need to rethink the meaning of *in situ* measurements for hydraulic properties. Often measurements (e.g., on a core sample) essentially represent properties at a point in space. Pressure testing results give properties in the so-called cone of influence. Using such property data on flow and

transport over a region of much larger scale needs to be done with care, with prediction needs or application requirements in mind. For example, predicting the future average ground water pressure head at a site would probably require much less stringent consideration than predicting the maximum concentration of contamination at a downstream location.

While it is useful to develop new measurement techniques, new instruments, and new computer codes, a careful rethinking of the entire procedure of field measurement, interpretation, and modeling-prediction (and their interplay) is needed, in the context of the objectives of such a site-specific study.

Quantitative Assessment of Uncertainties and Confidence Levels

It is well known that uncertainties in parameter values lead to uncertainties in modeling results, and various methods have been developed to handle this problem. Similarly, various stochastic methods have been advanced to assess the uncertainties caused by heterogeneity in properties that cannot (and probably should not) be measured in detail deterministically. In the context of predictive hydrogeology of a site, a number of other less well-defined uncertainties need to be considered. Examples include:

- *Uncertainties introduced by data density.* In the development of a structural model of a site (the conceptual model), geological, geophysical, and borehole studies are carried out. Areas of the site with the most measurements tend to have more structures, e.g., faults and fractures, than areas with fewer measurements. This is entirely an artifact of varying data density, which could introduce significant uncertainties in predictions.
- *Uncertainties related to structures, model size, and boundary conditions.* It has been recognized that the conceptual (structural) model is critical for predictive

modeling. A missing structure, such as a subhorizontal fault zone with possibly no surface manifestation, may have significant impact on the prediction of flow and transport at the site. Further, even if all the structures have been identified, their dip and strike directions and their continuity into the depth below ground are all factors that could impact hydrogeologic predictions. What are sometimes overlooked are the effects of model sizes and boundary conditions used in the predictive simulations. A small model size will automatically cut off long flow lines around the site, and these long flow lines may have significance for long-term predictions into hundreds of thousands of years. Further, the boundary conditions need careful consideration, because they may be transient over this time frame as well as spatially varying along a boundary. How to handle these kinds of uncertainties is an interesting research issue.

- *Uncertainties in combining uncertainties from different sources.* For studies of a site, we have not only geologic and hydrologic information, but also hydrochemical data and rock stress data. It is important to ensure that all the data are consistent with each other. For example, the presence of high-salinity regions should be consistent with the flow field measured at the site and the paleohydrological information. Another example is the dependence of fracture permeability as a function of depth below the land surface. Simple consideration argues that it should decrease, because of the increase in rock stress with depth. Further, because rock stress is a tensorial quantity, it will introduce anisotropy in fracture permeability, which also varies with depth. Inconsistencies among these multidisciplinary data need to be identified and understood, and their impact assessed. Methods also need to be developed to handle coupled uncertainties in multi-disciplinary information and to evaluate uncertainties in model predictions.

The above are just examples; research is needed to identify other sources of uncertainties, as well as reducing uncertainties as much as possible, by conducting reasonable additional measurements or by redefining the predictive quantities required. It is quite reasonable for society to accept and act on predictions with

uncertainty. Indeed, predictions should never be given without uncertainty ranges. Confidence level is quite another issue. You can make a prediction with a wide uncertainty range and yet have a high confidence level that the reality will be within this range. Work has been done to assess confidence levels by studying the past history of the so-called natural analogues; see for example, EC (2002). In general, how to assess confidence levels is still very much an open, but important question.

Remarks on Hydrogeological Education

Considering the emphasis on the need for predictive hydrogeology, it is useful to comment briefly on educational preparation. Generally, conventional geology education is not sufficiently quantitative and provides inadequate mathematical training, e.g., in analytical or numerical modeling. On the other hand, conventional civil engineering education does not provide adequate training in the physical insight needed for studying open, natural geological systems that include many uncertainties and variabilities. The need for rigorous mathematical training in a hydrogeology educational program is beginning to be recognized and addressed in a number of universities. However, training programs for physical insight, and for dealing with geological variabilities and uncertainties, are much more difficult to design. Students in good universities today are often well-trained in problem-solving in clearly defined problems, but are often wanting in dealing with ill-defined problems of open systems. They need to be trained not only to solve problems, but to question the definition of problems and whether the objective of a problem itself should be modified to be answerable by hydrogeology. Perhaps inclusion of courses in systems engineering and decision analysis would be helpful.

Another area of education that needs to be strengthened is “Quality Assurance” or QA. In its proper meaning, QA is to ensure transparency and traceability, and is actually just good scientific practice. At the most elementary level, this training is done by learning to write “good laboratory notebooks.” However, such training for laboratory notebooks has

not been much emphasized in recent years. Furthermore, the need for training in writing “good modeling notebooks” also exists. Often students are happy to be given some input parameters, go through the mechanics of modeling, and obtain the results. It would be a good training if the students are required to ensure that the input parameters are specifically referenced and can be traced back to original data, and, further, that the quality and applicability of these input data have been evaluated. One reason that QA has not been emphasized up to now is that conventional hydrogeology modeling results are often for short-term applications of, say, 30 years (one would know if one were right or wrong in 30 years or less), and they can often be checked by independent modeling work. However, with the emphasis on predictions of hundreds of thousands of years into the future, and the great effort needed to conduct such predictive modeling, QA becomes very much necessary, and students should be trained in it.

Finally, with the need to conduct research on coupled processes occurring at a site, which involve hydrogeology, chemistry, geophysics, rock mechanics and biology, the breadth of student education also needs to be enlarged. Such a need for interdisciplinary research is also discussed by Hunt and Wilcox (2003) in the context of ecohydrology. They emphasize that true interdisciplinary research should be “tightly coupled research, in which [the] disciplines are equally involved in the formulation of research objective, design of the work plan and on-going interpretation”. Obviously, students cannot be expected to be proficient in all of the different fields, but they should be well educated in one or two areas and trained in how to interact and interface with the others. To design a training program for effective interaction and interface with areas not in one’s own expertise is an open problem. Yet this skill is critical, because a multi-disciplinary team is often required to solve problems of importance to the society.

In summary, to train students in hydrogeology for participation in work addressing major problems that require long-term predictions, a fundamental rethinking of hydrogeological education is needed. New approaches are required for training in physical insight, critical thinking, uncertainty and risk analysis, and QA methods, as well as familiarity, in varying degrees, with mathematical techniques, geological processes, chemical and

biological complications, and system engineering. In addition to improved regular university programs, we may consider complementing them with specially designed courses and summer schools organized by consortia of universities in cooperation. The use of short courses and web-based learning courses may also be considered, especially for working hydrogeologists and engineers.

Concluding Remarks

The need for long-term hydrogeological predictions in solving some of today's key problems of concern to society has provided impetus for consideration of new hydrogeological research directions. Several areas of research beyond conventional, narrowly based research topics are discussed; namely, multiple couplings of *in situ* physico-chemical processes, the interplay between site characterization and predictive modeling, and quantitative assessment of uncertainties and confidence levels. Many scientific issues in these areas are yet to be resolved. Finally, a rethinking of hydrogeology educational strategy is needed at the university and postgraduate levels. In this sense, hydrogeology is an exciting field of research, with many challenges and opportunities.

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