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TRANSPORT MODELING - TECHNICAL AND LEGAL ISSUES

by

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TABLE OF CONTENTS

TRANSPORT MODELING - TECHNICAL AND LEGAL ISSUES

I. Introduction

Transport modeling is the process of representing the transport of dissolved species in groundwater systems. Modeling can be achieved by a variety of analogues, including physical models, electrical models, and numerical models; the great majority of transport modeling undertaken today uses numerical methods.

A model is an analog, usually a simplification, of a real-world process. Solute transport is an inherently complex process, so that an analog can be of great assistance in understanding the nature of that process, and of the past and future behavior of the system being modeled. Solute transport analogues are used, as are most analogues, for a range of purposes:

a. Hindcasting, or the estimation of past conditions, given present conditions. Hindcasting is frequently used in legal matters, where the conditions which existed in the past may be critical to the establishment of the possible extent of injury to property or health.

b. Forecasting, or the prediction[1] of future conditions, given past and present conditions. Forecasting is very often used in environmental evaluations, particularly when attempting to evaluate the likely outcomes of taking some (or no) action with respect to groundwater contamination.

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[1] I am reminded of an observation once made by a weather-person: "A prediction is part-way between a forecast and a prophecy: it lacks the scientific rigor of the former, and the divine guidance of the latter".

c. Establishing the nature of transport processes. In this mode of usage, the observed conditions in the groundwater system are compared with conditions predicted by an analog. If the analog and the actual conditions are coincident, then it is reasonable to conclude that the concept embodied in the analog is a reasonable representation of the real system.

II. Solute Transport

A. Principles

To understand solute transport modeling, it is necessary to understand something of the nature of solute transport itself. The transport of dissolved species in groundwater systems has been studied extensively for a very long time. Solute transport in groundwater systems is controlled by three principle processes: convection, dispersion, and retardation.

1. Convection

Movement of the dissolved material by the groundwater flow itself is called convection. The fundamental theory of groundwater flow is deceptively simple: it is explained by Darcy's law:

$$Q = K\ i\ A \qquad [1]$$

where: Q = flow rate $[L^3T^{-1}]$
K = hydraulic conductivity $[LT^{-1}]$
i = hydraulic gradient $[LL^{-1}]$
A = area $[L^2]$

The velocity of flow in a groundwater system is given by the rate of movement of the water. From Darcy's Law, the real average velocity of flow of water is given by:

$$V_a = K\ i\ /\ n_e \qquad [2]$$

where:
V_a = actual (average) velocity of water $[LT^{-1}]$
K = hydraulic conductivity $[LT^{-1}]$
i = hydraulic gradient $[LL^{-1}]$
n_e = effective porosity $[L^3L^{-3}]$

Thus the velocity of water is a function of the hydraulic conductivity, the hydraulic gradient, and the effective porosity of the medium through which the water flows. The flow of water takes with it, to a lesser or greater extent, the dissolved solutes.

2. Dispersion

As the water moves through the subsurface medium, it is subject to small or large scale subdivision of flow within the subsurface flow system; this process is described as dispersion. Dispersion results in the spreading of the flow paths for the water, and hence for any materials that are dissolved in the water. This process is generally described in probabilistic terms, with the lateral and longitudinal dispersion of the flow being described as follows:

$$\sigma_l = \sqrt{(2\ \alpha_l\ V_s\ t)} \qquad [3a]$$

$$\sigma_t = \sqrt{(2\ \alpha_t\ V_s\ t)} \qquad [3b]$$

where:
σ_l = standard deviation of concentration along flowpath $[L]$
σ_t = standard deviation of concentration across flowpath $[L]$
α_l = longitudinal dispersivity $[L]$
α_t = transverse dispersivity $[L]$
V_s = solute velocity along flowpath $[LT^{-1}]$
t = time $[T]$

The result of dispersion in solute flow is that an originally small area of concentrated solute will spread during flow and dispersion to be an oval shaped zone, with concentrations less than the original concentration, and with a bell-shaped concentration distribution.

3. Retardation

During the passage of a solute through a real geologic medium, the solute is usually at least partly removed from the groundwater by physical and chemical processes, most importantly adsorption by the material through which the solute is moving. This process is generally described in solute transport evaluations by the term retardation. By this is meant that the result of the physical and chemical removal and adsorption processes is that the solute appears to move less quickly than the water. The normal method of describing this is by the use of a retardation factor:

$$R = V_a / V_s \qquad [4]$$

where: R = retardation factor [-]
V_a = velocity of movement of groundwater [LT^{-1}]
V_s = velocity of movement of solute [LT^{-1}]

Using this factor, the final equation for the velocity of the solute is given by combining equations [2] and [4]:

$$V_s = (K\ i) / (n_e\ R) \qquad [5]$$

where: V_s = velocity of movement of solute [LT^{-1}]
K = hydraulic conductivity [LT^{-1}]
i = hydraulic gradient [LL^{-1}]
n_e = effective porosity [L^3L^{-3}]
R = retardation factor [-]

B. The Behavior of Real Transport Systems

Based on the above, the hydraulic conductivity (K) controls the quantity of water and dissolved solute that flows in a groundwater system, and also controls the velocity at which that flow occurs. It follows from this observation that in real groundwater transport systems, the great majority of water and solute moves in that small percentage of the total subsurface domain which exhibits the highest hydraulic conductivity, and the velocity of flow in that material is much greater than the average velocity of flow in the system. Put another way, the process of solute transport is inherently and importantly dominated by the heterogeneities of the system through which the flow occurs. This matter turns out to be critically important for the entire science of modeling of solute transport.

Some of the corollaries of this observation are that:

a. To understand solute transport systems, it is necessary to understand the nature of the heterogeneity of the system.

b. The longer solute is transported in a system, the more likely it is that it will encounter a highly permeable zone, and move along it rapidly. Thus the velocity of a groundwater transport system would be expected to increase with distance travelled, and the solute would be expected to travel on fewer and fewer major conduits in the groundwater system.

c. Average conductivities, concentrations, and other parameters are of little use in the evaluation of solute transport: transport is dominated by non-average conditions.

These matters dominate the issues that are of technical and legal concern in the use and abuse of solute transport modeling.

III. The Process of Modeling

A. General Description

It is difficult to evaluate a transport model without a knowledge of the process which modelers go through in the construction and use of such a model. The fundamental steps which are taken in modeling are development of a conceptual model, operationalization of the conceptual model, validation of the model, and use of the model. These steps are described in more detail below.

B. Development of a Conceptual Model

At the heart of modeling is the development of a concept of the flow and transport system which is of interest. The normal process used to develop a conceptual model is to assemble the geologic, hydrogeologic, and chemical information available to describe the flow and transport regime operating at the site. From this a concept of the natural system that produces the observed behavior can usually be deduced. It is this concept that forms the conceptual model. Generally, a conceptual model comprises the geologic setting of the transport system, and the hydraulic and transport properties of the materials making up that geologic setting.

C. Operationalizing the Conceptual Model

The conceptual model is transformed into a predictive tool by being operationalized. This is the process of taking the concept, and creating an analog which behaves in the same way as the conceptual model. In recent years this process has been achieved mostly by use of computer codes, which allow an analog of the real system to be developed within a numerical analysis system[2]. In general, the operationalization of a conceptual model involves the construction of a representation of the real geological system of the zone of interest, using hydrostratigraphic units, and the application of the significant hydraulic and solute transport parameters to those units. To make the analog ready for operation, it is also necessary to apply boundary conditions of flow and solute movement, and to prescribe an initial condition for the model.

D. Verification, Calibration and Validation of the Model

A model is only a technical construct until it is tested in some fashion against the system which it is intended to analog. This is an often inadequately performed step which is critical to the development of confidence that the model does indeed provide a usable predictive analog of the real system. There are three processes which are ideally required to demonstrate that an analog is reasonable: verification, validation and calibration.

1. Verification

Verification is the evaluation that the computer code that is being used does indeed perform the numerical computations correctly. This demonstration is normally accomplished by having the computer code evaluate a set of standard problems for which the

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[2] A clear distinction should be made between a model, which is the analog, and the computer code which operationalizes it, which is limited to the framework for analysis. There has been a tendency in the groundwater industry to describe a computer code as a model, which is incorrect in the terminology of this paper. There has also been a tendency to concentrate on the codes used for computer analysis of models, rather than the models themselves. In the experience of the author, almost all modeling errors stem from inappropriate development and operationalization of conceptual models of transport systems, rather than inappropriate selection of computer codes for that operationalization.

correct results are known (generally because there is an algebraic solution), and comparing the computed results with the known results. In general this is included in the development of a computer program, and is part of the normal quality assurance system for the code. Verification on its own does not guarantee that the model is reasonable; it simply ensures that the code correctly performs the computations correctly.

2. Validation

Ideally, a model will be validated. Validation is the process of demonstrating that the model successfully analogues the real behavior that is being modeled. The process of validation involves the development of the model, the application of the known parameters that control the model (principally the hydraulic conductivity, storage coefficient, porosity, dispersivities, and the retardation factor for each element of the model), the application of the boundary conditions, and the running of the model under a known set of conditions. If the set of conditions cover the range of conditions for which the analog is to be used, and the computed results for the flow and solute movement are the same as the actual behavior of system, then the model is validated for use under these conditions. This is rarely achieved, but is a powerful demonstration of the validity of the model.

3. Calibration

The process of calibration is the usual method of demonstration that a model is an effective analog of a real system. In this process, all the known information about the system is used to construct the conceptual model, parametric information is applied to the model for areas where it is known, and the known boundary conditions are applied. The model in this state still has many areas requiring further definition before it can be used as an analog of the real system. In order to complete the model, unknown parameters and boundary conditions are estimated, and the model run for a known set of conditions that have been observed in the real situation. The unknown model parameters are then adjusted until the results of the model (the groundwater flow and solute transport behavior, generally quantified by head, flow, and concentration) are reasonably similar to observed values of these variables in the real system. When and if a reasonable fit between observed and modeled results are obtained, the model is said to be calibrated for this kind of perturbation.

E. Use of the Model

Once the model has been constructed and either validated or calibrated, it is ready for use. Ironically, the actual use of the model for the purposes of evaluation is generally the easiest and least time-consuming activity in the entire modeling process, and is frequently somewhat anti-climactic for the modeler. The boundary conditions are set to represent the perturbation that is being modeled, and the model generates the results of that perturbation. In many cases, transport modeling is performed in two phases:

a. A flow evaluation, where the groundwater heads and flows are developed.

b. A transport evaluation, where the movement of the solute is computed, using the conditions developed in the flow evaluation.

In general, the time dependency of the problem is principally the result of the movement of the solutes; the transient behavior of the groundwater flow system is usually rapid when compared with the rate of movement of the solute.

IV. Technical Issues in Transport Modeling

The process of modeling is complex, and it is relatively easy for the modeler to incorrectly model a solute transport situation. The sources of modeling errors are plentiful. This section discusses the technical issues that must be appropriately considered if the results of solute transport modeling are to be reliable for the uses to which they are put.

A. Analog Issues

A model is not usable for prediction unless it is a reasonable analog of the behavior that is being evaluated or used. In order for an analog to be effective, it must exhibit the following qualities:

1. Predictive power

The model must behave in the same, or in an acceptably similar way, to the real system of which it is an analog. The difficult part of this requirement is the term "acceptably". It is rare for exact verisimilitude to be required of a model. In general, only a limited range of the real behaviors of the system are actually of interest. As long as the model satisfactorily mimics those behaviors, its performance on the remainder of the behavior of the system is in general unimportant from a technical point of view[3].

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[3] From a legal point of view, however, the credibility of a model may be attacked if its performance is poor as an analog for matters not of direct interest in the matter for which it is being used. As a general matter, in litigation it is generally wise to use a modeling approach that reasonably mimics the entire system, even if only a small portion of the model is actually used in court.

2. Uniqueness

In order for a model to be credible as an analog, it is necessary for it to be unique. That is, there should be enough information that it is not possible to create two different models which can be calibrated against the information, yet when used as a predictive tool, produce solute transport predictions which are substantially different[4]. In real application, no model is in fact unique; there are thousands of choices of input variables, and thousands of degrees of freedom in the typical analysis. Fortunately, however, this is not usually a major problem. Experience with the use of models suggests that, providing that there is a sufficient body of information to define the model, and a sufficient body of information against which to calibrate the model, there is only one credible model that provides reasonable calibration against the information, and thus the predictions which are made by the use of this model are generally reliable, at least for a reasonable extrapolation into the past or future.

3. Representativity

A model must represent the groundwater and solute transport in ways that appear reasonable. It is conceivable that a model could produce an acceptable match with past behavior, yet be inappropriate for forecasting or hindcasting because the calibration does not represent the changed conditions which are involved in the period to be modeled. This is a common problem, and can only be overcome by ensuring that the calibration/validation process includes perturbations to the system which are similar to those which are to be modeled.

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[4] "Substantially different" in this context means that the different results would lead a decision-maker to reach different conclusions, depending on which analog was used. For example, two different modeling approaches to the same problem might, if they were non-unique, lead to a different choice of remedial action in an environmental contamination evaluation, one choice being appropriate, and one perhaps being inappropriate.

4. Simplification

The degree of simplification that is included in a model is a source of great difficulty. In practice, a modeler is constantly torn between including as much detail as possible in the model, for fear of omitting a feature which may turn out to be critical to the result, and omitting detail, so that the modeling process is tractable in terms of analysis time and information demand. Any model must be a simplification; the complexity of any natural system in detail defies an exact analog[5].

The most critical simplification choice which occurs relates to the representation of the variability of hydraulic conductivity. As noted above, the rate of solute transport that occurs in real systems depends heavily on the highest conductivity materials. Accordingly, great error can be injected into an analysis if the conductivity is averaged too heavily: this will generally result in predictions of solute transport being considerably slower than the real behavior, and the area which the model predicts will be impacted considerably greater than the real impact area.

B. The Porosity Issue

Porosity is the volume of the permeable material that is not taken up with rock or soil particles. In a saturated material, it is the space that is available for groundwater flow, and solute transport. The water flows through the voids, and not through the solid material. The effect of porosity (n_e) on the velocity of solute transport is shown in Equation [5]: the higher the porosity the lower the velocity of solute transport.

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[5] While this is true, direct testing of real systems, as an alternative or an adjunct to modeling, is a preferred method of evaluation of groundwater transport systems if it can be done in a time and cost-effective manner.

In the case of sands, about ⅔ of the cross sectional area for flow is taken up with essentially impermeable silica particles. Thus the velocity of the water is about 3 times as fast as would occur if the flow were taking place in the same cross sectional area without the sand. If the same material were rock, say a granite, then the flow would have to take place in the cracks between rock blocks, known as the joints. The total volume of voids in this case is much less, often considerably less than 1% of the total volume of the rock. Accordingly, the velocity of the water in the actual voids (the cracks) would be 100 times the rate that would occur in the same cross sectional area without the rock material.

In general, however, not all the voidspace or porosity in a material is equally available for transport. Some of the voids may be locked up in the interior of blocks of solid material: a good example of this is the voidspace in vesicular basalt, which comprises bubbles of gas in an essentially impermeable material. This voidspace does not participate in groundwater flow or in solute transport. In other cases, the material may exhibit dual porosity, in which the porosity within blocks or zones of the material may be less accessible than the porosity on the periphery of the blocks. A good example of this may be fractured sandstone, where the porosity comprises perhaps 1% in the fractures between sandstone blocks, through which solutes move rapidly, and 25% in the interior of the blocks, through which water moves much more slowly, due to the higher porosity.

Clearly the modeling of real materials requires some knowledge of the nature of the porosity, which is experimentally very difficult. Computer codes which allow the modeling of dual porosity materials, which represent both the rapid and slow movement described above, are still in their infancy, and demand information about the nature of flow which is difficult to provide based on current testing techniques. However, making assumptions about the nature of the porosity which ignores either of the styles of porosity can lead to models which may represent some aspects of the transport behavior, but which ignore other critical aspects. Finally, in general averaging of these behaviors is not likely to be effective, as this may result in the model not representing either aspect successfully, and therefore producing a model which cannot be calibrated.

C. The Dispersion Issue

As noted in the discussion in the previous section, dispersion causes solutes dissolved in groundwater flow to spread out, taking up more area, and moving both faster and slower than the average velocity of the groundwater in which they are dissolved. The process is a result of the fact that the groundwater constantly divides to flow round grains, rock blocks, or to take advantage of local high permeability zones. If the conductivity of the pathways available to the flow is sufficiently distinct, and there are relatively few different materials, it may be possible to model each pathway separately, thus leaving the modeling of dispersion to microscopic subdivisions, the effects of which are relatively well known. However, in general the dispersion parameters (see Equation [3]) are used in modeling to accommodate the heterogeneity in the system at all but the largest scale, so that they become a calibration factor to allow for all kinds of dispersive behavior.

This practice distorts the picture for solute transport. The dispersion only changes the way in which the contaminant spreads out in the groundwater system. The centroid of the solute mass remains unchanged by dispersion, so that the overall transport of solute is not changed. In real situations, however, the high conductivity conduits not only cause some of the solute to be transported more quickly than the rest, but they also act as principal conduits for flow, or drains for the system. Thus the further a solute moves in a groundwater system, the more likely that it is to be drawn to one of the few highly conductive conduits in the system, and thereafter move more quickly than the average conductivity of the material would suggest. Any model which uses dispersion to mimic this behavior will probably be a poor analog of the long term behavior of the system. Put another way, calibrating such a model against the observed behavior to date is likely to underestimate the rapidity and distance that the solute will move in the future.

This phenomenon is probably the reason that the dispersivity parameters in Equation 3 have been found to vary for a given model; they essentially depend on the distance that the plume has moved. The longer the travel distance, the higher the dispersivity that is required to successfully model the plume. This finding suggests that the modeling of the movement of the plume using classical dispersion is flawed, and that the use of dispersivities to provide an analog of the effects of heterogeneity is not an adequate modeling approach. Unfortunately the alternative is to be aware of, and to include in the model, a rather detailed understanding of the real heterogeneity of the hydrogeologic system. In general neither the investigation nor available computational power allow more than the coarsest representation of the real variability in even the simplest real systems. As a result, the power of current solute transport tools for extrapolation of solute movement into the future is relatively poor.

D. Chemical Issues

1. Retardation

As noted in Section II of this paper, the movement of solutes in groundwater systems is driven by the movement of water. The extent to which the solute moves with the water is affected by interactions between the solute, the water, and the environment through which the water moves. The practice in the evaluation of the modeling of solute transport is to lump all such interactions under the single term "retardation", but this is often an over-simplification, and sometimes a critical error.

Classically, retardation is the result of a single phenomenon, adsorption of solute onto, or into, the particles of material through which the solute passes. The process of adsorption generally involves attachment of solute ions to the surface of a solid phase material. The process is generally reversible, and after a period of time the solute ion will detach from the solid material, and once again move through the groundwater system. The ensemble effect of the detachments is that the solute moves more slowly through the solid medium than the groundwater. As noted in Equation [4], the retardation is defined in terms of the relative velocities of water and solute.

Retardation is a function of the nature of the solute, the nature of the solid phase material through which the groundwater moves, and the concentrations of other solutes in the system. It is relatively easy to determine the retardation factor in the laboratory, provided a sample of the soil and of the groundwater which will be flowing through it is available. When the phenomenon is indeed classical retardation (that is it is reversible adsorption), then the laboratory values for retardation generally provide a good analog; when other factors are "lumped" into retardation, then frequently the analog is poor.

2. Chemical Processes

In addition to adsorption, there are other processes that have the ability to modify the concentration of a solute in a groundwater system. These processes include chemical reactions, dissolution, precipitation, and coprecipitation. In general, most solute transport models do not evaluate their effects, except to assume that they can be modeled by the use of a retardation factor. In general they cannot, for the following reasons:

a. Reactions. Chemical reactions frequently are irreversible: the solute involved in the reaction ceases to exist, and in general new solute species are generated as a result of the reaction. Proper modeling of this cannot be achieved by the assumption that the solute is merely adsorbed, and can desorb at any time. The result of such an assumption on the results is to over-estimate the future concentration of the solute, and to under-estimate the future concentrations of the product materials. This is normally significant in the modeled system.

b. <u>Precipitation and dissolution.</u> Precipitation and dissolution of materials constitute physical processes that can change solute concentrations in groundwater, but which differ importantly from adsorption. Whether a species precipitates or dissolves is controlled mainly by the concentration of this and other species in the solution. If a solute precipitates, then the concentration of the solution remains constant at the solubility limit of the solute until all of the precipitate has been re-dissolved. This behavior is distinctly different from retardation, and the use of retardation as a substitute for this behavior will in general cause an over-estimate of concentration of the solute in the liquid phase, and an under-estimate of the time that removal of the solute from the system (remediation) will take. These errors may be significant with respect to environmental decision making, particularly in the selection of chemical remedies for contamination of groundwater.

c. <u>Kinetics.</u> The rate of reaction between a solute and the material through which it flows, or the interaction between solutes in two different solutions, may be quite slow, due to the rate of reaction at the temperature of the groundwater. Adsorption theory assumes that there will be equilibrium between the solid phase and the liquid phase solute. If this does not occur, then the retardation that is expected will not occur fully either, thus introducing error into the computation of solute transport. The result of this error in modeling will in general be to under-estimate the movement of solutes, and to over-estimate the extent to which remedial actions will be successful.

In summary, modeling of chemical processes other than adsorption by the use of retardation is likely to introduce error, particularly in the estimation of future concentrations of solutes, and in the evaluation of the effectiveness of remedial actions. Most of the errors are unconservative in respect of impact and effectiveness of cleanup.

There are a number of computer codes that have been developed which consider physico-chemical reactions other than adsorption. While these models are currently in the nature of research tools, it appears that in the reasonably near future they will gain usage in the environmental and the legal process. The models consider all flow and chemical processes, and produce a very accurate analog of the chemical interactions between solutes and solid phase materials. The disadvantage of these codes is that they require an overwhelming amount of information in order to operate, and require the largest computers known for successful simulation of real flow and chemical systems. A further disadvantage is that they are essentially uncheckable.

E. The Code Issue

There are a large number of available codes for the evaluation of solute transport problems. Most of these codes have been developed with a specific type of problem in mind, and are to that extent specific. Codes can be identified by reference to literature or by application to a variety of organizations that act as clearinghouses for code sales.

It is not the purpose of this paper to evaluate codes, nor to provide a listing of available codes. However, as noted above, most of the codes available today perform the computational task of groundwater flow and solute transport correctly, and to that extent are almost all fundamentally acceptable. Code choice comes down, for the most part, to personal preference of the modeler, and the nature of the problem to be solved.

V. Legal Issues

The complexity of the natural system involved in solute transport, and the sophistication of the modeling codes and data assemblages needed to reasonably simulate these systems, creates difficulties when the results of such modeling are used or evaluated. This is particularly true when model results are presented to lay or non-technical audiences, which is frequently the case in legal matters involving contaminant transport. The legal issues which arise are the result of the technical issues: they relate generally to comprehensibility of the modeling process, and accuracy and credibility of modeled predictions.

A. Technical Acceptability of a Model in Litigation

Expert opinion in court cases involving solute transport matters is often guided by, or assisted by, the results of solute transport modeling. If the modeling can be supported as reasonable, then it appears that there is no reason why the results of modeling should not be admissible as part of the basis for the development of the expert opinion. However the reliability of the results of forward or backward extrapolation by solute transport modeling has been shown above to be potentially poor, except with the most sophisticated model, being operationalized by the most robust code. In the opinion of the author, the key to solute transport modeling being admissible evidence lies in satisfying the following objectives:

a. <u>Appropriate calibration.</u> The model must be calibrated against a range of conditions for which information is known, and which are relevant to the perturbations that are expected in the period to be modeled. The extent of the calibration period, and the quality of the fit between the modeled and the real data provides a measure of the quality of the predictive power of the model.

b. <u>Reasonable extrapolation.</u> The shorter period that a model is used for extrapolation, the more likely that the results are going to be reliable. Ideally the calibration period is of the same order of time as the proposed extrapolation, either forward or backward. By the time that the extrapolation is beyond 10 times the calibration period, except in special cases it is likely that the results are more speculative than probative.

c. <u>Credible results.</u> The results of any modeling activity have to be able to be checked for credibility. In general, this requires an alternative analysis of the key features of the computation, in order to develop a "ball-park" result for evaluation against the computer results. Once this reasonableness check has been performed, there are relatively limited methods of checking the results: benchmarking (that is, running the problem using another code, to show that the result is not dependent on the code); physical modeling; and field testing. However these last two options are limited: generally the modeling is being done in the first place because there is no direct test opportunity available.

Ultimately the test for a model to be acceptable in litigation is whether it is reasonable. This reasonableness depends on:

a. the model being based on a reasonable interpretation of the data available to construct it (an acceptable conceptual model);

b. the analog of the model being appropriately represented in the computer idealization of the system;

c. the boundary conditions and perturbations that are applied to the analog being consistent with the real situation;

d. the model being successfully tested against real, well documented field information that is relevant to the evaluation being conducted; and

e. the predictive runs of the model encompassing the reasonable bounds of the real situation.

B. Effectiveness of Modeling in Litigation

Even the most reasonable, credible model is not of utility if the court cannot understand the basis for it, or cannot interpret the results. As discussed above, at its core, solute transport modeling is technically complex. However the success of modeling in demonstrating the likely behavior of solute transport systems will ultimately depend on the comprehension of the judge and/or jury to which the information is presented. The following aspects appear to be important in conveying modeling information in this situation:

a. Use of graphics. A picture in modeling is truly worth a thousand words. Because of the quality of computer graphics, the entire results of a modeling simulation can, and should, be presented graphically. This saves the trier of fact from having to wade through pages of numbers which are extremely difficult to comprehend.

b. Demonstration of extrapolation. The presentation of model results should illustrate the extent to which real information is available to support the case, and that the modeling provides infill information, rather than providing the entire basis for the conclusions in the matter at trial. This can be done by overlaying the results of the model on the results obtained from the field, to show that where both results sets exist, they agree.

c. Demonstration of uniqueness. Some attempt should be made to avoid the suggestion of "knob twiddling", where the modeler may be able to get any answer desired by simply varying some of the unknown parameters of the analysis. This can be done in a variety of ways, but some analysis of the sensitivity of the results to assumptions, and the effective presentation of these results, may be necessary to avoid this common, and often correct, criticism of predictive modeling.

VI. Conclusion

The modeling of solute transport processes is often the only practical method of providing an appreciation of the unobserved behavior of contaminant transport systems in the past, or their expected behavior in the future. The actual behavior of such systems is complex, and is generally dominated by a relatively small proportion of the groundwater flow system in which the transport takes place. Because of the technical complexity and sensitivity of the real system, credible modeling of these systems is demanding. Technically successful solute transport modeling depends on appropriate model conceptualization, construction, calibration, and utilization.

Effective use of models for hindcasting or forecasting the behavior of solute transport systems in a litigation context requires conveying to a lay audience the nature of a complex technical process, and the meaning of the results of that process. This requires that the credibility of the model needs to be established by addressing the technical issues described in this paper. The challenge of effectively conveying the modeling validity and results can be assisted by the use of graphical presentation of the calibration of the model, and of the results of the model when used to provide unmeasured past behavior of the transport system, or to predict future behavior of the transport system.