Advanced Sensing Technologies Reduce Uncertainty and Risk in Transport Modeling and Remediation Strategies

By

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CRITICAL NATIONAL NEED IDEA

BACKGROUND:

Recent advances in diagnostic measurement technology have had major impacts on many fields, especially in medicine. Physicians are now able to engage procedures that in the past were of extraordinary risk, yet today are routine because they have validated information prior to and during surgery. Similar advances have been made in aerospace, where materials and systems are pushed to their near limits to achieve mission success. Again, such capabilities are possible through better quantitative diagnostic knowledge that is coupled with predictive models to assess performance envelopes.

This TIP submission explores that potential impact on the nation if similar advances were made in the field of water transport, especially groundwater. The hydrologist wants quantitative vector data for input into physical models of transport. Direct property data for hydraulic conductivity and assessment of vector flows would have a dramatic impact on how the country monitors and manages groundwater. The ability to cost-effectively characterize vector flow in reasonable time periods will dramatically impact the cost of planning remediation. Such data generated in hours or minutes (instead of days, weeks, or months for conservative tracers) and representing flow measurements integrated over realistic distances, will rewrite site planning and outcomes. The economic and environmental impact of such a breakthrough will literally alter the landscape.

Current technology can only provide limited information as to dynamic transport of *water and solutes* through the ground. Typical systems in use today depend on a variety of measurements, yet do not provide broad quantitative input to models. Two examples of current practices are injection of tracers or hot water, with subsequent monitoring of dispersion. In each technology, there is valuable information gathered but not what is required to directly enter into hydrodynamic models. For example, in hot water injection, the innate heat transfer of the base material is an unknown variable that propagates errors in the analysis. Injection of tracers introduces an undesirable variable into the flow and the interpretation of the data can be influenced by the local conductivity at the injection site, leading to errors in the predictive model results.

Other technologies that have been applied to this problem include colloidal particle tracking and acoustic Doppler technology. The particle tracking does not generate vector information and the requirement of a well can alter the very flow that is to be measured by creating a mixing volume. As with injection technology, the specific localized conductivity can influence the data requiring multiple measurements over numerous sites to assess average parameters. Aquifer pumping tests, slug tests, and measurement of synoptic water levels as indirect measurements, can all have significant errors and logistical difficulties (e.g. managing large volumes of contaminated water for pumping tests).

If a groundwater sensor system can be developed that provides significant improvements over current state-of-the-art, it will have national impact. The value of such a development enhances the quality of our models, reduces the cost of acquiring groundwater flow parameters and can provide near real time feedback for operations such as aquifer pumping to alert managers of impending concerns. Other applications of such a sensor system may have direct value to assessment of earthen dams for stability, for leeve systems for leakage and subsidence, and for high topography areas for impending mudslides.

State and local governments, as well as most Federal agencies, have significant knowledge gaps regarding quantitative assessment of the heterogeneity of an aquifer, essential to properly characterize solute transport in groundwater. State and local governments do not have the funds and ability to develop more cost-effective advanced sensing tools that would eliminate the knowledge gaps. The National Science Foundation Sensors and Sensing Systems (SSS) program supports academic research on methods to acquire and use sensor data on civil, mechanical, and manufacturing systems. However, the SSS program is targeted towards academic research, *whereas this TIP proposal integrates academic research, and recognized leaders in transitioning science to engineered solutions, through a unique university and private industry partnership.*

HYDROLOGIC OPPORTUNITY:

Ground-water resources in many parts of the United States are severely stressed by human activity [1]. Despite the importance of knowing the heterogeneity of an aquifer in order to properly characterize solute transport, this goal remains elusive [1]. Furthermore, small-scale sensors that can measure velocities and tracers in three dimensions may lead to advancements in understanding surface-ground water interactions, which are particularly essential in wetlands. Wetlands are vulnerable to contaminant fluxes; yet, offer buffer-zone benefits in hurricane-prone coastal areas.

Over the past several decades many different models for surface and subsurface contaminant transport, under varying conditions and assumptions, have been proposed and tested. These range from models based upon very simple, one-dimensional analytical (closed form) solutions, which assume a completely homogeneous and isotropic fluid (or porous medium in the case of subsurface models), to complex three-dimensional numerical codes that allow for complete specification of flow and contaminant characteristics throughout a three-dimensional grid.

For any complex set of models, two key questions would be:

(1) to what extent can this set of codes accurately predict all of the essential complex physical, biological and chemical phenomena?

(2) given the accuracy of this set of codes, is it reasonable to make regulatory decisions based on either short-term or long-term predictions?

Strictly mechanistic models, particularly those applied to simulate complex water quality processes, are usually inadequate and sometimes inappropriate for use as the basis for management decisions. A thorough uncertainty analysis has never been successfully undertaken for most of the complex models. All of these flow and contaminant transport models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes, and so can provide only an approximation of the actual spread of a contaminant from a given site and the associated risk. This situation presents a familiar, yet difficult problem to the analyst and the decision-makers. Sufficient data are rarely, if ever, available to apply the most complex, three-dimensional contaminant transport models to a monitored site. The analyst must, whether explicitly or implicitly, choose a transport model based on a trade-off between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models.

Even with the choice of an appropriate transport model, considerable uncertainty is likely to be present in the analysis of contamination risk. For example, in groundwater solute transport models (which require estimation of parameters which are difficult to measure and spatially variable, such as hydraulic conductivity and dispersivity), there is often good reason to doubt the accuracy of the input data. For instance, if an analytical model requires the spatial average of the hydraulic conductivity throughout the local area of the aquifer, and the available data consist of only one or two slug tests, plus perhaps an expert opinion, there is good reason to doubt that the reported best estimate of the parameter accurately reflects the true mean value.

Uncertainty enters the modeling process in three ways:

(1) through natural parameter variability;
(2) through measurement error, which also introduces uncertainty in parameter estimation; and,
(3) through model error, representing uncertainty introduced by the degree to which the simplifying assumptions used to develop a model fail to accurately represent the actual physical, biological and chemical processes at the site in question.

This uncertainty propagates itself throughout the analysis, such that the proposed remedial measure strategies may also be risky. The first two of these sources of uncertainty can be analyzed separately. The third source of uncertainty in the analysis is due to the degree to which the transport model applied may misrepresent actual processes at the site. This source of uncertainty is very difficult to quantify, and indeed may be impossible to quantify for specific sites unless extensive sampling and monitoring is carried out.

An alternative is to collect accurately measured field data to reduce the level of uncertainty. The most cost-effective means of reducing such uncertainty is to **accurately measure ground water velocity** (in addition to measuring ground water levels, a much easier task). There is ample evidence in the literature that variability in the hydraulic conductivity introduces the largest amount of uncertainty into the modeling process. Groundwater flow can be described with Cartesian tensor notation as:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_i}\right)=S_S\frac{\partial h}{\partial t}+W \qquad (1)$$

where K_{ij} is the hydraulic conductivity of the porous media (a second-order tensor) (*L/T*), h is the hydraulic head (*L*), S_S is the specific storage (*1/L*), t is time (*T*), W is the volumetric flux per unit volume (*1/T*), x_i are the Cartesian coordinates (*L*), and the summation convention of Cartesian tensor analysis is implied. The term in parentheses is the velocity vector (directly proportional to the hydraulic conductivity and the hydraulic gradient), which is used in the *advective-dispersive-decay* equation below. Inverse modeling techniques can be used to better estimate the hydraulic conductivity.

For saturated groundwater, solute transport in an incompressible fluid flowing through a porous medium can be described with the same convention as:

$$\frac{\partial(\varepsilon C_g)}{\partial t}+\frac{\partial(\rho_b \overline{C}_g)}{\partial t}+\frac{\partial}{\partial x_i}(\varepsilon C_g V_i)-\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C_g}{\partial x_j}\right)-\sum C'_g W+\lambda_g(\varepsilon C_g+\rho_b \overline{C}_g)=0 \qquad (2)$$

where ε is porosity, C_g is volumetric concentration in the fluid (*M/L³*), ρ_b is the bulk density of the aquifer material (M/L^3), $\overline{C}_g$ is the mass concentration of solute sorbed on the solid of aquifer material (*M/M*), V_i is a vector of interstitial fluid velocity components (*L/T*), D_{ij} is a second-rank tensor of dispersion coefficients (L^2/T), W is a volumetric fluid sink or source rate per unit volume of aquifer (*1/T*), C'_g is the volumetric concentration in the sink/source fluid (M/L^3), and λ_g is the decay rate (1/T).

Although many of the variables identified above are subject to the errors introduced by natural variability and by measurement technique (e.g., gradient, dispersivity, hydraulic conductivity, etc), it is the natural variability of hydraulic conductivity [13 orders of magnitude] that propagates the largest amount of uncertainty. Through advanced small-scale sensors that can measure velocities and tracers in three dimensions, this high level of uncertainty can be reduced and result in a much better characterization of aquifer heterogeneity.

Current methods for measuring groundwater flow do not fully meet the needs of groundwater modeling efforts, nor do they provide the efficiency of real-time data collection [2-3]. In particular, most available methods are not suitable for 3-D vector flow characterization and are restricted to a narrow range of soil media. Consequently, site remediation decisions are often based on incomplete groundwater flow information at best, or inaccurate information at worst. For example, tracer injection techniques are invasive and can be time consuming and expensive, and as a result are often not employed. Colloidal borescope methods can only measure horizontal flows at a point, so they provide incomplete information [4]. Thermal sensors are also point measurements and are limited for use in unconsolidated sands and are unreliable at low velocities [5-8]. In addition, each of these techniques represents point measurements rather than an integrated measurement between two well sites, which is more accurately used in computational data inversion.

<u>POTENTIAL ECONOMIC IMPACT</u>:

The potential identified in the “Hydrologic Opportunity” section embraces far more than scientific validation of models. That alone is of significance, but in the tough economic times we are facing, the ability to dramatically improve projections is a critical enabler for decision makers who will have to prioritize projects based on information. This TIP topic has the potential to reduce errors in projections by providing ground truth to guide those who develop models and those who depend on model outcomes to serve the public.

Although the actual number of contaminated sites in the United States is unknown, estimates of the total number of sites with soil and contaminated groundwater may be as high as 300,000 to 400,000. Recent estimates for cleaning up these sites over the next 30 years have ranged as high as $1 trillion (National Academies Press, 1997) [9]. The Department of Defense (DOD) alone has identified nearly 6,000 sites at its facilities that require groundwater remediation and has invested $20 billion over the past 10 years to clean up these sites [10]. Many of the challenges and significant costs of contaminant remediation are related to field site characterization. Conventional techniques for measuring hydrogeologic parameters typically involve drilling boreholes and either retrieving soil and/or groundwater samples for further analysis, or utilizing borehole logging techniques. Overall, measurement of groundwater flow by currently available techniques can be costly, time-consuming, incomplete, and invasive, potentially causing disturbance of the very in-situ conditions of interest that need to be measured. Because of these issues, measurements are typically sparse in relation to the volume that they are intended to represent. Many measurements recover information about only a very small volume of the shallow surface associated with either the size of the core sample or some limited zone around the borehole. Natural heterogeneity exhibits variability over a wide range of scales and hence is difficult to characterize due to scarcity of measurements and scales associated with conventional field sampling techniques. The limitations of current methods therefore result in making remediation decisions and designing remediation systems based on incomplete, and potentially inaccurate data.

Assuming that site characterization represents only 5% of a cleanup project's life cycle cost, estimates for money spent on characterization at DOD sites approaches $1 billion, and could be as high as $50 billion based on the NRC estimate. These costs do not include the direct and indirect costs associated with incorrect cleanup decisions, and worse exposures of contaminants to ecological and human populations.

Development of advanced sensing technologies that are able to provide near-real time, direct measurement of three-dimensional groundwater flow would be invaluable to the environmental community [11]. Groundwater flow and contaminant transport data would be collected in a matter of days, as opposed to weeks or months using conventional approaches. Also, the use of advanced sensing technology would minimize the generation and management of secondary waste (e.g. contaminated groundwater). Most importantly, the data generated would be of superior quality and resolution compared to that generated by conventional approaches. This would allow for the ability to make regulatory decisions based on predictive output from groundwater models, with much less uncertainty than is currently possible.

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