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IN SEARCH OF REPRESENTATIVENESS: EVOLVING THE ENVIRONMENTAL DATA QUALITY MODEL

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Environmental regulatory policy states a goal of "sound science." The practice of good science is founded on the systematic identification and management of uncertainties; i.e., knowledge gaps that compromise our ability to make accurate predictions. Predicting the consequences of decisions about risk and risk reduction at contaminated sites requires an accurate model of the nature and extent of site contamination, which in turn requires measuring contaminant concentrations in complex environmental matrices. Perfecting analytical tests to perform those measurements has consumed tremendous regulatory attention for the past 20–30 years. Yet, despite great improvements in environmental analytical capability, complaints about inadequate data quality still abound. This paper argues that the first generation data quality model that equated environmental data quality with analytical quality was a useful starting point, but it is insufficient because it is blind to the repercussions of multifaceted issues collectively termed "representativeness." To achieve policy goals of "sound science" in environmental restoration projects, the environmental data quality model must be updated to recognize and manage the uncertainties involved in generating representative data from heterogeneous environmental matrices.

INTRODUCTION

Investigating and restoring contaminated sites face conflicting goals: Site decisions are supposed to be protective and based on sound science, yet project costs are expected to be low. Conflict arises since gathering environmental data to support these kinds of decisions is generally expensive because measuring trace chemicals in complex, heterogeneous matrices can be extremely difficult. Developing the technologies and expertise for trace contaminant analyses challenged analytical chemistry to create the new discipline of environmental analysis, with new techniques and new equipment. A natural outcome was intense

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legal and regulatory attention on the reliability of chemical analysis. Meanwhile, the high per-sample cost of analysis naturally drove cost-conscious project managers to sharply limit the numbers of samples. Unfortunately, the heterogeneity of most environmental matrices raises fundamental uncertainties about the ability to extrapolate analytical results from a few small-volume samples to the much larger volume of matrix being investigated. Cost and practical considerations have blunted awareness within the environmental community to the fact that sample representativeness is the foundation of data quality. Now that analytical methodologies are more advanced, sampling is generally recognized as the largest single source of uncertainty in environmental data. But for many years, there were few ways to escape the quandary of how to ensure data representativeness on behalf of good science and correct environmental decisions while at the same time containing project costs.

Fortunately, that situation has changed. Ongoing technology advancements in rapid soil and groundwater sampling tools, field-portable analytical instrumentation, and decision-support software present both opportunity and challenge. It is *now* possible to manage the critical sampling and decision uncertainties that stem from the heterogeneity of waste-related matrices. In addition, cost-effective generation of data in "real-time" (often, but not always, involving field analytical methods) permits a work-flow strategy commonly known as "dynamic work plans," which employs real-time decision-making in the field by experienced staff following pre-approved decision trees. When thoroughly planned and properly implemented, real-time decision-making saves 30–50% of project costs because fewer remobilization cycles (to fill data gaps) are required, and expensive equipment and labor (such as backhoes, drill rigs, and their operators) are more efficiently utilized. Dynamic work plans also produce more thorough and accurate site characterizations because immediate feedback allows data gaps and unexpected discoveries to be rapidly resolved. The resulting complete and accurate conceptual site models enable decision-makers to design successful and cost-effective treatment systems and redevelopment options.

The obvious benefits of these new technologies and dynamic work plan strategies are gradually increasing their acceptance by regulators and practitioners. Yet many institutional barriers remain that challenge the environmental cleanup community to evolve their assumptions and paradigms, as well as their mechanisms for contracting and regulatory oversight. For example, field methods are often dismissed as "field screening" and are not used to their full potential. Many practitioners find it difficult to access the appropriate technical expertise needed to design sampling and analytical plans capable of generating data of known and documented quality that is explicitly matched to the intended project decision. Communicating concepts that are fundamental to managing data uncertainty is difficult because the historical data quality paradigm begins and ends with the assumption that environmental data quality is a function of the analytical method. This paper discusses evolution of the environmental data quality model by evaluating the relationship between data quality and decision quality, and by distinguishing analytical quality from data quality. A "next-generation" data quality model can create the framework needed for explicitly managing both data and decision uncertainties using new strategies to produce greater decision confidence ("better"), while simultaneously shortening project lifetimes ("faster") and cutting overall project costs ("cheaper") more than ever before possible (Refs. 1–3).

"QUALITY" AS A POLICY GOAL

Exhortations for "sound science" and "better quality data" within the context of regulatory environmental decision-making are increasingly popular. Is the current data quality model sufficient to achieve sound science? Is "data quality" really the key issue, or is there something more fundamental at stake? Although this paper focuses primarily on contaminated site cleanup, many of these issues are broadly applicable to other areas of environmental management.

Since 1979, U.S. Environmental Protection Agency (EPA) policy has required an Agency-wide quality system, with the goal of providing "environmental data of adequate quality and usability for their intended purpose of supporting Agency decisions" (Ref. 4). Yet the linkage between data quality and data usability for decision-making is easily lost from programmatic and project planning and implementation. "Data quality" is too often viewed as some independent standard established by outside arbiters independent of how the data will actually be used. Project managers tend to follow a checklist of "approved" analytical methods as the primary means of achieving "data quality." Yet, striving for "high quality data" under the current model has proven to be an expensive and sometimes counterproductive exercise.

In contrast to checklist approaches to "data quality," sound science in regulatory and project decision-making is achieved by acknowledging and managing decision uncertainty. Correspondingly, acceptable data quality is achieved by managing all aspects of data uncertainty to the degree needed to support the decisions for which the data are intended. Managing uncertainty, either of decisions or of data, requires careful planning using relevant expertise and technical skills. Calls for “sound science” and “better data quality” are meaningless without a simultaneous commitment to include scientifically qualified staff when planning science-based programs and projects. Environmental programs exist because there is work that must be done at the project level. Policy-makers that desire to see sound science in environmental decisions need to provide a coherent vision that will steer the development of program infrastructure that focuses on managing *decision quality* at the *project* level.

It is a mistake to assume that scientific data are (or can be) the only basis for regulatory decision-making. Science may be able to provide information about the nature and likelihood of consequences stemming from an action, but the *decision* to pursue or reject that action (i.e., accept or reject the risk of consequences) based on scientific information is within the province of values, not science. Even the choice of how much uncertainty is tolerable in statistical hypothesis testing lies in the realm of values. Thus, it is appropriate that many non-scientific considerations feed into a regulatory decision-making process. This does not invalidate a foundation of “sound science” as long as the various roles of science and values are differentiated, and any underlying assumptions and other uncertainties in both data and decision-making are openly declared with an understanding of how decision-making could be affected if the assumptions were erroneous.

DECISION QUALITY AS DEFENSIBILITY

The term “decision quality” implies that decisions are defensible (in the broadest scientific and legal sense). Ideally, decision quality would be equivalent to the correctness of a decision, but in the environmental field, decision correctness is often unknown (and perhaps unknowable) at the time of decision-making. When knowledge is limited, decision quality hinges on whether the decision can be defended against reasonable challenge in whatever venue it is contested, be it scientific, legal, or otherwise. Scientific defensibility requires that conclusions drawn from scientific data do not extrapolate beyond the available evidence. If scientific evidence is insufficient or conflicting and cannot be resolved in the allotted time frame, decision defensibility will have to rest on other considerations, such as economic concerns or political sensitivities. No matter what considerations are actually used to arrive at a decision, decision quality (i.e., defensibility) implies there is honest and open acknowledgment and accountability for the full range of decision inputs and associated uncertainties impacting the decision-making process.

Managing scientific defensibility is extremely difficult when the science behind a new initiative is immature. This was undeniably the situation when Superfund and other site cleanup programs were created in the 1980s. In a classic chicken-and-egg dilemma, fledgling waste programs were asked to create site investigation and cleanup procedures despite the fact that the scientific and technical foundations for those procedures barely existed. At the same time, programs were called upon to legally defend their cleanup decisions. To develop the needed scientific theory, practice, and tools for measuring and mitigating contamination and its effects, the government began to pour funding into research to understand the complex relationships among environmental, chemical, and health phenomena. Despite the immaturity of the science, policy-makers and the public expected that cleanup activities would begin and proceed immediately. Few anticipated the daunting technical complexities that would be encountered by cleanup programs as they leapt into this unknown sphere of science and engineering.

FIRST-GENERATION STEPPING-STONES THAT BECAME STUMBLING BLOCKS

When immediate action is desired, but knowledge and expertise are not yet sufficient to plot the smartest plan of attack, a reasonable tactic is to initially create a consistent, process-driven strategy based on the best available information so everyone can "sing from the same sheet of music" while experience and knowledge are being accumulated. Certainly this made sense for the emerging cleanup programs. To be consistent with sound science, however, such a process-driven approach should be openly acknowledged by all participants as the *first* approximation that it is, with the understanding that one-size-fits-all oversimplifications will be discarded in favor of more scientifically sound information as it becomes available. Although science may be comfortable viewing first approximations as short-lived stepping-stones subject to continual improvement and revision, this view is less welcome when economic and litigious forces intersect with broader societal goals in a regulatory crucible. This is one of the fundamental conflicts faced by policy makers seeking "sound science" as a basis for regulation. Furthermore, as individual cleanup programs proliferate at the state and local levels, first approximations become more and more solidified in bureaucratic processes that naturally prefer predictability and consistency. First approximations take on the aura of "received truth." Disseminating and integrating new information and procedures becomes difficult. The net result is that the regulatory and procedural infrastructures that support project implementation have trouble keeping up with maturing science.

A prime example of this kind of lag is the prevailing concept of "data quality" as applied to environmental analytical chemistry data. A universal assumption of the current model is that analytical quality is equivalent to data quality. Since definitive analytical methods offer the *potential* to produce very high analytical quality (it is debatable whether the achieved analytical quality is as good as assumed when rote environmental methods are used indiscriminately for certain analytes and complex matrices), conventional wisdom has it that any data produced by screening analytical methods are automatically inferior and suspect. Therefore, technologies such as *in situ* or field analytical methods risk rejection simply because they do not fit the ancestral data quality model. The point of this paper is that it is this data quality model that is inferior and suspect, since it was developed as a first approximation based on incomplete knowledge of environmental systems and limited technology capability. At the root of the current data quality model are several assumptions about environmental chemical analysis:

1. "Data quality" is determined by the accuracy and documentation of the chemical analysis procedure (traditionally performed in a laboratory).
2. The accuracy of analyses on environmental samples can be ensured by consistently performing all analyses according to strictly prescriptive regulator-approved methods.
3. Analytical uncertainty (i.e., the degree to which the accuracy of the analytical results are in question) can be managed according to a checklist regimen of quality control procedures that rely largely on ideal matrices such as reagent water or clean sand to establish method performance.
4. Laboratory quality assurance is equivalent to, and substitutable for, project quality assurance.
5. With "cook book" analytical procedures for the laboratory, and a list of approved analytical methods in hand during project planning, the need for environmental analytical chemistry expertise can be minimized in the environmental laboratory and eliminated from project planning.

Decision-makers accepted these assumptions when establishing site investigation and cleanup procedures and programs, even though scientists warned of their questionable validity (Refs. 5, 6). This oversimplified "analytical quality equals data quality" model supported the imperative to "define the nature and extent of contamination," itself a first approximation of a regulatory-based sampling and analysis strategy for hazardous waste sites. It was hoped that "defining the nature and extent" would produce information (in the form of data) that would tell the project manager what to so with the site. Naturally, it was impossible in the early days to predict the kind of cleanup and land reuse decisions that would be faced later on, so each site had to be a "study" with ill-defined and shifting project goals. There was no choice but to collect data with the hope that it would be appropriate to making site decisions once it became clear (1) what those site decisions would be, and (2) how defensible those decisions would have to be to gain the buy-in of regulators or stakeholders. This unfocused approach *can* work as long as there are sufficient resources (time, money, and stakeholder forbearance) to repeatedly return to the site to fill each newly discovered data gap as piecemeal identification of individual site decisions (and their attendant uncertainties) progresses on the way to site closure. There is no doubt that that strategy was the best available *at that time*.

But fortunately, advancing knowledge, technology, and 20-plus years of experience means that this process can be replaced by something better. It is possible now to anticipate project goals (or at least a short-list of desirable site outcomes) at the start of the project. Regulatory agencies provide residential and industrial thresholds derived from estimations of human health risks and other impacts to the environment as targets for decision-making. Vast institutional knowledge exists for most site types, their contaminants' release patterns, and exposure scenarios. To be sure, we have only scratched the surface in our understanding of contaminant behavior, risk, and cleanup options, but we no longer need to function as if we must start from scratch for every project. In fact, as program budgets shrink and rapid reuse of sites is desired (e.g., in "Brownfields" programs), the traditional approach is no longer viable due to its cost and inefficiency. "Defining the nature and extent" without first identifying project goals amounts to groping around in the dark. It carries a serious danger that decision uncertainties will not be identified in a timely manner, and that data generation designs will be inadequate to defend the decisions being made. If there are not sufficient funds to continue data collection until decision uncertainties are managed, there is a strong incentive to downplay or ignore decision uncertainties. This in turn increases the chance that decision errors could pose unacceptable risks to receptors, or will waste resources through ineffective remedial actions (Refs. 7, 8). This is the antithesis of sound science.

EVOLVING A SECOND-GENERATION DATA QUALITY MODEL

To set the stage for an updated data quality model, we must clarify the term "data quality." According to EPA's Office of Environmental Information, data quality is "the totality of features and characteristics of data that bear on its ability to meet the stated or implied needs and expectations of the user/customer" (Ref. 9). What data users "need," ultimately, is to make the correct decisions. Therefore, data quality cannot be viewed according to some arbitrary standard, but must be judged according to its ability to supply information that is representative of the particular decision that the data user intends to make. Said in a different way, *anything* that compromises data representativeness compromises data quality, and data quality *should not be assessed except in relation to the intended decision* (Ref. 10). The assumptions of the current data generation model and routine application of this model to environmental decision-making for site cleanup are inadequate to ensure that data are representative of the site decisions being made. The root cause of data non-representativeness is the fact that environmental data are generated from environmental samples (i.e., specimens) taken from highly variable and complex parent matrices (such as soils, waste piles, sludges, sediments, groundwater, surface water, waste waters, soil gas, fugitive airborne emissions, etc.). This fact has several repercussions:

1. The concept of representativeness demands that the scale (spatial, temporal, chemical speciation, bioavailability, etc.) of the supporting data be the same (within tolerable uncertainty bounds) as the scale needed to make the intended decisions (does unacceptable risk exist or not; how much contamination to remove or treat; what treatment system to select; what environmental matrix to monitor; what analytes to monitor for; where and how to sample; etc.). In contaminated site projects, the true state (such as the concentrations of contaminants across space or time or the properties of the matrix that control contaminant fate and transport) can easily vary markedly over smaller (inches to feet to yards) or larger (feet to yards to miles) scales that depend heavily on one's perspective. Decisions about risk and treatment design also vary over a range of scales. High variability at one scale may be inconsequential if viewed over a different scale. Discrete contamination patterns (such as "hotspots") may be apparent at some scales, but not at others. Since it is not resource-feasible to characterize the "true state" of all relevant properties of the site at all possible scales, there must be a rationale to decide which scale(s) is(are) important. The purpose of project planning is

to develop an understanding of the scale over which decision-making (e.g., risk decisions, remedy selection, remedy design) will occur, identify what uncertainties need to be resolved in order for defensible decision-making to occur, and then design a data generation scheme that will provide the corresponding information to manage those uncertainties. That is how sound science is practiced. Without first defining the decision, selecting the scale over which to "define nature and extent" becomes guesswork.

2. The concept of representativeness can be coarsely broken into sample representativeness and analytical representativeness, both of which are critical to managing data uncertainties:
   - Sample representativeness includes procedures related to specimen selection, collection (i.e., extraction from the parent matrix), preservation, and subsampling (although this is often included with "analytical" since it typically takes place in the lab). All are crucial to data quality, but the representativeness of specimens is difficult to ensure without sufficient sampling density to understand the scale and characteristics of matrix heterogeneities. Even perfectly accurate analysis is no guarantee of good data quality if the sample were not representative of the properties of concern to the decision-maker. Since many environmental matrices are highly heterogeneous on many different scales that affect contaminant concentration and behavior in analytical and biotic systems, most of the uncertainty in most of today's site data stems from the sampling side, although inaccurate analysis certainly can (and do) occur.
   - Analytical representativeness involves selecting an analytical method that produces test results that are representative of the decision. Causes of analytical non-representativeness include selecting the wrong method or erroneously interpreting method results (such as selecting a method that reports total DDT-related isomers when a regulatory decision based on 4,4′-DDT is required). Analytical representativeness is compromised when matrix interferences degrade method performance to the point where erroneous decisions would be made if the data were not recognized as suspect. If interferences are found, sound science demands that method modification or an alternate method be used to compensate. However, not infrequently regulatory programs inhibit the use of alternative methods that could improve method performance. Evaluating analytical performance on ideal matrices (reagent water and clean sand) provides little reassurance that equivalent performance is being achieved on project-specific samples. Well-behaved matrices provide valuable

information about analytical quality, but data users cannot automatically assume that their performance is representative of analytical quality for the real-world matrices under investigation.

3. The wide range of decisions, contaminants, matrices, and interferences encountered in site cleanup programs and the pace of technology development make it impossible for prescriptive analytical requirements to accommodate the multitude of complex and interacting variables that determine method performance. Regulatory flexibility for the selection and operation of analytical methods is not only vital to ensuring representative results, but also fosters acceptance of highly cost-effective, second-generation technologies and strategies.
4. The scientific and technical complexities of site cleanup require that appropriate scientific expertise be involved in up-front project planning (to identify decision goals and design data collection strategies), in design implementation, and in data interpretation. *Without appropriate expertise, identification and management of relevant heterogeneities and uncertainties does not occur, data quality is frequently mismatched to data use, and sound science is not achieved.*
5. Arbitrary regulatory requirements for "data quality" should be avoided since this short circuits the planning process needed to achieve sound science. Regulations should focus on requirements for performance that demonstrate explicit management of decision uncertainty.
6. Conceivably there will be circumstances where it is more cost-effective to manage the uncertainty involved in ensuring a protective outcome by simply choosing the most protective action without generating data. Generating the data needed to manage decision uncertainty may cost more than simply taking action. Although there may still be uncertainty about whether the decision to take protective action is correct in an absolute sense, the ultimate goals of the decision-making process will have been achieved.

In contrast to the assumptions that underlie the current data quality model, a second-generation data quality model for the environmental field will explicitly recognize that:

- Data quality is an emergent property arising from the interaction between the attributes of the analytical data (such as its bias, precision, detection and quantitation limits, and other characteristics that together contribute to data uncertainty)

and the intended use of the data (which is to assist managing decision uncertainty).
- Data uncertainty is comprised of both sampling and analytical uncertainties.
- Analytical uncertainty in a test result arises from both the analytical uncertainty of the measurement method itself *and* from interaction between the sample matrix and the analytical process. The analytical uncertainty arising from the method *itself* is only a fraction (and often a negligibly small fraction) of the overall data uncertainty. The impact of sample matrix on analytical uncertainty varies to a greater or lesser degree depending on how well the analytical methodologies have been matched to the characteristics of the particular sample matrix and to the data needs. Complex environmental matrices are notorious for interferences that degrade analytical reliability. Current quality assurance practices may not detect when interferences are causing problems if there is not a high index of suspicion on the part of the analyst and the data user.
- Sampling uncertainty accounts for the majority (and in some situations, nearly all) of the data uncertainty. This uncertainty can be managed by increasing the sampling density and/or by targeting sample collection designs to yield the most valuable information (i.e., gather more data where decisions are more uncertain, such as boundaries between “clean” and “dirty” areas, and less data where there decisions are more certain, such as obviously “clean” or obviously “dirty” areas). Sample representativeness requires that all aspects of sampling design be matched to the scale of decision-making.
- Procedures to estimate and report data uncertainties (e.g., uncertainty intervals) to the data user need to be developed for the environmental field.
- Investment in properly educated and experienced technical staff is a necessary and cost-effective means to achieve data quality and good science where numerous complex and interacting variables must be evaluated and balanced.

SUMMARY

Years of experience with investigating and cleaning contaminated sites have made it clear that data quality cannot be managed independent of the overarching goal of decision uncertainty management. Pursuing arbitrary notions of “data quality” becomes an elusive, aimless, disconnected resource sink that fails to achieve sound science.

Data quality (management of data uncertainty) and decision quality (defensible management of decision uncertainty) are distinctly different endeavors, both of which are critical to the pursuit of sound science. Yet their roles are easily confounded in the regulatory arena. Isolated attempts to address data quality issues that fail to recognize and address fundamental conflicts between outdated models and contemporary scientific knowledge only perpetuate problems and stakeholder dissatisfaction. Pursuing policies based on sound science will challenge regulatory agencies to modernize first-generation environmental models and regulatory strategies to accommodate the ever-evolving progressive nature of science itself.

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