

October 1, 2001

ENVIRONMENTAL Science & Technology

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*Managing
Uncertainty* in
Environmental
Decisions

**Ionic Liquids:
An Industrial
Cleanup Solution**

**Design of
Natural Gas Pipeline
Questioned**

PUBLISHED BY
THE AMERICAN
CHEMICAL SOCIETY

Managing Uncertainty in **Environmental Decisions**



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**Applying the
concept of
effective data to
contaminated sites
could reduce
costs and
improve
cleanups.**



U.S. EPA

Many environmental decision makers and practitioners worldwide assume that the quality of data pertaining to a contaminated site is primarily determined by the nature of the analytical chemistry methods used to collect information. This assumption, which diminishes the importance of sampling uncertainties, can have a pronounced, negative effect on the cost and effectiveness of contaminated site cleanups.

Data produced by regulator-approved laboratory analytical methods are commonly assumed to be practically free of uncertainty and so are termed “definitive data”. In contrast, data produced in the field are generalized as “field screening” and are considered too uncertain to support important project decisions or regulatory actions. One of the reasons for such generalizations is that the current regulatory mindset does not readily distinguish between analytical methods and the data produced by them. Although the assumptions behind this mindset are inaccurate, they are pervasive enough to inhibit the widespread adoption of better strategies for assessing and restoring contaminated sites.

We propose that a more comprehensive understanding of data quality concepts can improve decision making for site investigation and cleanup projects. Defensible decision making is only possible when the concept of data quality is understood to encompass all of the parameters that influence contaminated site management data, not just analytical method performance.

As a basis for managing the “bottom line”—decision uncertainty associated with site cleanups—environmental practitioners need to better balance their management of both sampling and analytical uncertainties. There would be greater confidence in site management and cleanup decisions if field analytical methods were perceived as primary tools around which work strategies are designed to manage the overall decision uncertainty, rather than just as less expensive substitutes for traditional laboratory analyses. The following discussion explains how the use of field analytical methods can improve data quality and the reliability of site management decisions, while lowering cleanup costs. We suggest the term “effective data” to describe this inclusiveness, which more com-

prehensively integrates sampling and analysis uncertainty management into the concept of data quality.

Context and terminology

Historically, regulators dealing with contaminated sites have insisted upon adherence to a limited list of approved analytical methods because of the common perception that the prescriptive use of methods assures defensibility and data quality. Whether the U.S. EPA restricts the selection of methods for waste programs is beyond the scope of this paper, but the reality is that responsible parties fear that regulators will automatically reject data if the methods used are not EPA-approved.

Practices based on this assumption actually degrade decision quality. In fact, relying exclusively on rigid requirements for contaminated site analyses may undermine the very scientific defensibility these programs hope to secure.

What does the term data quality really mean? Ambiguous usage in the environmental field has made this term rather nebulous, but it is fair to say that for the vast majority of regulators and professionals involved in site cleanup, acceptable data quality is equated with the use of EPA-approved analysis methods. It is assumed that definitive data are automatically produced when laboratories use definitive analytical methods and adhere to standardized quality assurance/quality control (QA/QC) (1).

Defining data quality along these lines leads to numerous logical inconsistencies and contradictions, as well as requirements for process (i.e., use of regulator-approved analytical methods) rather than outcome (i.e., reduced decision uncertainty). Options for analytical method selection and implementation are artificially limited, while laboratories are held responsible for environmental data quality. As a result, efforts to improve data quality invariably center on increasing laboratory oversight, rather than on developing mechanisms to manage the largest sources of uncertainty in data, which are issues related to sampling. This same mindset sees screening analytical methods as producing screening-quality data, uniformly considered inferior to conventional laboratory data, which creates an immediate bias against their use for decision making.

Misperception about data quality will only be resolved when the concept is built on a solid scientific foundation. EPA took a significant step toward that goal when it recently clarified its definition of data quality to mean all features and characteristics of data that bear on its ability to meet the stated or implied needs and expectations of the customer (2). This was done to reflect performance-based regulatory goals and the realities of scientific data generation and use. EPA guidance further explains that "... data quality,

as a concept, is meaningful only when it relates to the intended use of the data. Data quality does not exist in a vacuum; one must know in what context a data set is to be used in order to establish a relevant yardstick for judging whether or not the data set is adequate" (3).

Defining data quality in terms of its ability to support defensible decisions avoids the distortions created when data quality is judged solely according to the analytical method used. The analytical method is

only one of many factors that impact

overall data quality. Analytical

chemistry data are gener-

ated on samples as

the output of an

orderly chain of

sequential ac-

tivities. The

quality of that

data depends

on the integrity

of each and every

step in the chain.

The single most im-

portant step is the first: se-

lection and collection of samples

that are representative of the feature(s) of

the parent material being investigated in the context

of the decision(s) to be made. A nonrepresentative

sample produces misleading information. Critical el-

ements of a sample's representativeness may include

the sample's physical dimensions, its location, and

the timing of collection. If representativeness cannot

be established, the quality of the chemical analysis is

irrelevant (4).

Other preanalytical activities, such as sample

preservation, transportation, storage, and subsam-

pling, further influence data quality. Sample analysis

is actually an umbrella term that groups several dis-

tinct activities, each of which may involve a different

analytical method such as sample preparation (e.g.,

extracting analytes from the sample matrix), cleanup

(reducing the impact of coextracted interferences),

introduction (presenting a sample or extract to an in-

strument), and determination (instrumentation that

generates the analytical results). The most reliable

environmental results are generated when options

for these methods are mixed and matched according

to the nature and composition of the sample, the tar-

get analytes, and the rigor of the desired results.

Finally, the analytical process and the results must be

documented and accurately transmitted to the data

user. Typically, analytical laboratories administer only

the last elements of the chain of activities and have

no way to control the representativeness or integrity

of the sample before it reaches them.

Because a problem in any single step of the chain

compromises data quality, project planners should

carefully consider each step in relation to how the re-

sulting data are expected to support the project goals

(5, 6). Even if the pitfalls of sample representative-

ness and preservation are avoided, the complexity of

samples encountered in waste programs (e.g., soil,

sediment, and waste materials and ground, surface,



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and waste waters) guarantees that ensuring analytical data quality is seldom a simple matter.

All analytical methods are potentially subject to interference by the physical or chemical constituents of the sample. The more complex the sample matrix, the more likely it is that interferences will cause significant analytical problems. It is unrealistic to expect to consistently produce cost-effective, reliable environmental data when regulatory requirements mandate uniform method selection and operating conditions without regard for site-specific considerations. Laboratories cannot assure reliable results if they are required to use methods inappropriate to the analyte or the matrix.

Prescriptive methods are scientifically feasible only when both the sample matrices and the decisions for which the data are to be used are known never to vary in ways that will affect either the reliability of the analysis or the interpretability of the results. This is not true in the real world and is why analytical flexibility is so important to assure analytical data quality in cleanup programs (7).

The desire of regulators to ensure the reliability of environmental data is commendable, but the current approach cannot achieve that goal. Not surprisingly, data quality problems continue to plague site cleanup programs (8). These problems will continue as long as “one-size-fits-all methods” turn “data quality” into a commodity to be purchased from the lowest bidder, a practice that has seriously undermined the sampling and analytical expertise of the industry.

Most regulators and practitioners are unaware that there are options for each step in the sampling and analysis chain and that the choice of option helps to determine overall data quality. For example, the discussion of analytical methods in project plans and reports seldom extends beyond specifying the instrumental determinative method (e.g., EPA SW-846 Methods 8260 or 8270). Analytical data quality cannot be adequately assessed by evaluating only the last step in the analytical chain. Of even greater importance is the fact that the major source of uncertainty in environmental data sets—as much as 90% or more by some estimates—is due to sampling variability as a direct consequence of the heterogeneity of environmental matrices. This is a major problem that needs to be addressed (9, 10).

Finding a better way

One-size-fits-all approaches cannot remedy the data quality problems associated with site cleanups nor the decision errors that can stem from them. Instead, greater decision confidence and significant cost savings over conventional approaches are being achieved using a work strategy we refer to as the Triad approach.

The Triad approach relies first on thorough, systematic planning to articulate clear project goals and encourage negotiations to determine the desired decision confidence. Only then can a multidisciplinary technical team determine what information is needed to meet those goals. A key feature of this planning is identifying what uncertainties could compromise decision confidence and allowing team members with appropriate sampling and analytical expertise to ex-

plore cost-effective strategies to minimize those uncertainties. Often, the most cost-effective work strategy involves the second leg of the Triad, which is using a dynamic work plan to make real-time decisions in the field. The third leg of the Triad is using field analytical methods to generate real-time on-site measurements that support the dynamic work plan.

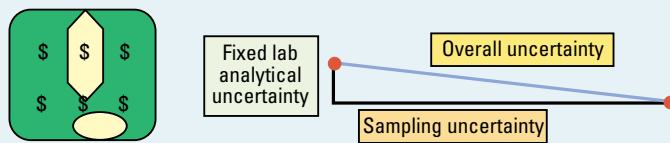
There are significant advantages to using this Triad approach. Projects managed using these concepts have demonstrated cost savings up to 50% over traditional management approaches that rely on repeated trips to the field to fill data gaps that become apparent only as laboratory results are interpreted weeks or months later after sampling (4).

Figure 1 depicts a conventional grid approach to sampling design followed by fixed laboratory analysis for a hypothetical site containing two idealized hot spots—locations with significantly higher contaminant concentrations than the surrounding area. The companion graphic is a highly simplified representation of the overall decision uncertainty as the vector sum of the sampling and analytical components. Figure 1 symbolizes the paradox that good analytical quality data *points* may actually form a poor quality data *set*, which produces misleading conclusions because budget constraints will invariably limit the number of samples for determining contamination. The overall uncertainty in environmental data is governed by its largest component, which field studies consistently find to be the uncertainty stemming from sampling considerations (10, 11). Thus, little is gained by stringently minimizing analytical uncertainty when sampling uncertainty is not addressed.

FIGURE 1

Conventional data quality approach

The overall uncertainty using a conventional approach to sampling and analysis is depicted for an idealized site having two hot spots. The accompanying triangle graphic (a simplified conceptual representation of relative uncertainties) indicates that the contributions to overall uncertainty from sampling and analysis can be described as a vector sum of the components, drawn here in a common 9:1 sampling:analytical ratio. Although the analytical uncertainty is minimized by conventional laboratory analysis, sampling uncertainty is not addressed because of the high per-sample costs. Note that as a result of the low-sampling density necessitated by high-sampling costs, one of the hot spots is not detected. Dollar signs (\$) denote sample results by more expensive, lower-analytical-uncertainty methods.



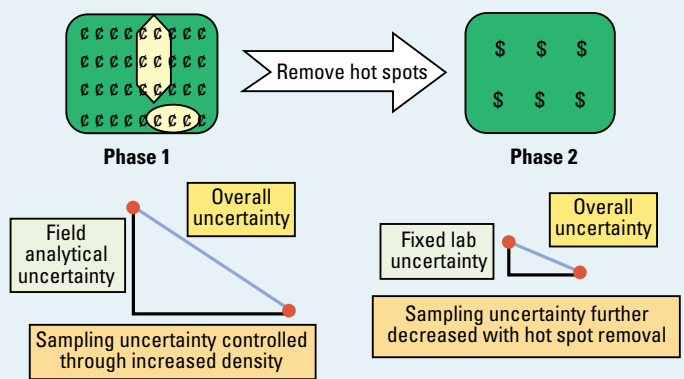
For the same idealized site, Figure 2 illustrates how using less accurate and less costly data points can improve overall data quality under the Triad approach. When analytical costs are lower, more samples can be analyzed, yielding more confidence in the representativeness of the data set (Phase 1). This is most effective if field methods are used to generate data points and a dynamic work plan rapidly resolves

any uncertainty about the location and volume of contamination (e.g., locate and delineate hot spots in a single field mobilization). If the analytical data quality used to manage sampling uncertainty is less than what is eventually needed to make final project decisions, such as whether the site can be declared “clean”, more expensive analyses may be performed on samples selected to accurately represent the feature of interest (Phase 2). However, if the initial method produces data of sufficient rigor to support defensible decision making, then additional, expensive analyses would be redundant and unnecessary.

FIGURE 2

Uncertainty management using the Triad approach

In Phase 1, analytical uncertainty increases so that unit sample costs decrease, allowing a higher sampling density than with the conventional approach. As a result, sampling uncertainty decreases, lowering the overall uncertainty in data interpretation. Phase 2 depicts how sampling uncertainty is further decreased if hot spot removal reduces the variability in contaminant concentration and if representative sampling locations for more rigorous analysis (if needed) are identified based on Phase 1 information. The vector representations (triangles) of uncertainty indicate that the overall uncertainty in the data set for site decision making will be much less than the overall uncertainty in the conventional data set shown in Figure 1. A dynamic work plan allows both phases to be performed in a single field mobilization. Dollar signs (\$) denote sample results by more expensive, lower-analytical-uncertainty methods, whereas cent symbols (¢) denote sample results by less expensive, higher-analytical-uncertainty methods.



Communicating information

The unifying theme of the Triad approach is managing the total decision uncertainty. This is also a crucial aspect of effectively using field analytical methods. Although not all field analytical technologies use screening methodologies (e.g., a field-portable gas chromatograph coupled to a mass spectrometer is a definitive analytical tool), many others do (e.g., immunoassays).

In general, data produced by screening analytical methods will contain more analytical uncertainty than data produced by definitive methods. However, this does not necessarily make definitive methods better than screening methods. Definitive methods are not foolproof; interferences or other problems can markedly increase their analytical uncertainty, especially when laboratories are not expected to mod-

ify procedures to accommodate matrix effects. On the other hand, the analytical uncertainty inherent to screening methods can be minimized by several strategies, including selecting appropriate QA/QC procedures to ensure that the data are of known and documented quality that is matched to the data's use (4). Most important, all field analytical technologies uniquely offer the ability to cost-effectively manage the largest single source of decision error—sampling representativeness.

There is a stark irony here. If the question of quality for contaminated site investigations and cleanups is framed in terms of the bottom line, then the ultimate goal is decision quality. Data quality should be judged according to whether both the sampling and analytical uncertainties in the data set(s) support decision making at the desired degree of decision confidence (3). It is not difficult to see that the intelligent application of screening methods supports robust data sets and a definitive (i.e., high quality) decision. In contrast, relying solely on regulator-approved, definitive analytical methods, while ignoring sampling uncertainty, easily produces screening quality data sets and uncertain decisions. Yet, whenever field analytical methods are used, even when some technologies are based on definitive analytical methods, both the process and the data are universally characterized as “field screening”. Obviously, this term is ambiguous and misleading. Therefore, we believe it should be discarded in favor of terms (e.g., on-site measurements or field-based analysis) that do not imply that data should be judged as screening quality simply because of where the analysis was done.

We propose alternate phraseology to reflect current EPA guidance that both sampling and analytical uncertainties must be managed in order to assess data quality guidance (3). We consider the two terms, effective data and decision-quality data, to be equivalent when describing data of known quality that can be shown to be effective for making defensible primary project decisions because both sampling and analytical uncertainties have been explicitly managed to the degree necessary to meet clearly defined project goals. No assumptions are made about whether definitive or screening analytical methods are used, only that relevant uncertainty is managed. Characterizing data (or the proposed design for collecting data) as effective for decision making is therefore only possible if the planning process explicitly articulates the project decisions with an expression of the associated tolerable uncertainty.

Although this definition of effective data (decision-quality data) may seem simple, there is much more that can be said about what the terms should encompass (4). Primary project decisions are usually those decisions that drive resolution of the project, such as whether or not a site is contaminated and what subsequent actions, if any, will be taken. Therefore, contaminant data are usually the data sets of interest. But data sets can interact in complex ways. For instance, a contaminant data set that might not be effective for making project decisions when considered alone might become effective when combined with other data or information that manage the remaining un-

certainties. We refer to these as collaborative data sets.

For example, a set of 230 data points generated by low-cost pesticide immunoassay (IA) kits plus a set of 40 data points generated by high-cost definitive organochlorine pesticide analysis could together comprise a collaborative data set that is effective for making project decisions about the cleanup of a small site with contaminated soil. The high density of IA data points manages sampling uncertainty by ensuring that no significant contamination escapes detection. Collaborative analysis of selected IA samples using a definitive method ensures that the analytical uncertainties inherent to the IA kits (a possible negative bias due to extraction inefficiency, a built-in positive determinative bias, and cross-reactivity to degradation products and other closely related compounds) are managed well enough to ensure that decisions based on IA results are either correct or err on the side of caution (protectiveness). Considered alone, neither data set would be sufficient, but together, they cost-effectively achieve highly confident site cleanup and closeout decisions (12).

Of course, there are many reasons for collecting data besides support of the primary project decisions. We use the term ancillary data to include, for example, data for worker health and safety monitoring, data that help the project team understand the fate and disposition of contaminants (such as meteorological or stratigraphic data), and data that aid decisions about the representativeness of environmental samples (e.g., groundwater turbidity). Because there may be multiple roles for certain data sets even within the same project, we expect that the boundaries between these data classifications (effective, collaborative, and ancillary) may blur. The label is less important than the concept that assessment of data quality must integrate both sampling and analytical aspects of data generation with their various uncertainties into the context of intended data use.

Emerging site characterization and monitoring tools can lower the costs of environmental restoration and long-term monitoring, but only if regulators and practitioners begin to incorporate them into modern, efficient work strategies, such as dynamic work plans. Field analytical technologies supply real-time data that make dynamic work plans possible and make rigorous management of sampling uncertainty financially feasible as a standard practice. Our decision-making paradigm and terminology embody a conceptual approach that reinforces the central theme of systematic project planning, which is management of decision uncertainty. This promotes EPA's recommendation to assess data quality according to the data's intended use in support of scientifically defensible environmental decisions.

Acknowledgments

Preparation of this paper was coordinated through EPA's Technology Innovation Office (TIO). TIO promotes the use of innovative technical tools and strategies for cleanup and reuse of contaminated sites. For additional details, refer to <http://clu.in.org>. Disclaimer: The mention of trade names is for identification purposes only and does not constitute an endorsement

by the U.S. EPA, the U.S. Army Corps of Engineers, or the authors. This article has undergone internal EPA review to verify consistency with existing EPA policy; however, the recommendations contained in this paper are solely those of the authors.

References

- (1) *Data Quality Objectives Process for Superfund Interim Final Guidance*; EPA 540-R-93-071; U.S. Environmental Protection Agency, U.S. Government Printing Office: Washington, DC, 1993.
- (2) *Office of Environmental Information Management System for Quality*; Final Version 1.3, U.S. Environmental Protection Agency, Washington, DC, 2000, Jan. 22, 2001.
- (3) *Guidance for Data Quality Assessment: Practical Methods for Data Analysis (QA/G-9 QA00 Update)*; EPA 600/R-96/084; U.S. Environmental Protection Agency, U.S. Government Printing Office: Washington, DC, 2000.
- (4) Crumblin, D. M.; et al. *Applying the Concept of Effective Data to Environmental Analyses for Contaminated Sites*; EPA 542-R-01-013; U.S. Environmental Protection Agency, U.S. Government Printing Office: Washington, DC, 2001 (<http://clu.in.org/tiopersp>).
- (5) Fairless, B. J.; Bates, D. I. *Pollut. Eng.* **1989**, *21* (3), 108-111.
- (6) Smith, R.-K. *Interpretation of Organic Data*; Genium Publishing Corporation: Amsterdam, NY, 2000.
- (7) *Test Methods for Evaluating Solid Waste, Physical/Chemical Methods*; U.S. EPA SW-846; U.S. Environmental Protection Agency: Washington, DC, 2001; Draft Update IVB, see chapter 2. (www.epa.gov/SW-846).
- (8) Office of Inspector General. *IG Audit Report*; E1SKF7-08-0011-8100240; U.S. Environmental Protection Agency, U.S. Government Printing Office: Washington, DC, 1998 (www.epa.gov/oigearth/audit/list998/8100240.pdf).
- (9) Homsher, M. T.; et al. *Environ. Lab.* **1991**, *1.3* (5), 10-14.
- (10) Jenkins, T. F.; Walsh, M. E.; Thorne, P. G.; Thiboutot, S.; Ampleman, G.; Ranney, T. A.; Grant, C. L. *Assessment of Sampling Error Associated With Collection and Analysis of Soil Samples at a Firing Range Contaminated With HMX*; Special Report 97-22; U.S. Army Corps of Engineers/Cold Regions Research and Engineering Laboratory, National Technical Information Service, Springfield, VA, 1997 (www.crrel.usace.army.mil/techpub/CRREL_Reports/reports/SR97_22.pdf).
- (11) Jenkins, T. F.; Grant, C. L.; Brar, G. S.; Thorne, P. G.; Ranney, T. A.; Schumacher, P. W. *Assessment of Sampling Error Associated With Collection and Analysis of Soil Samples at Explosives-Contaminated Sites*; Special Report 96-15; Army Corps of Engineers/Cold Regions Research and Engineering Laboratory, National Technical Information Service, Springfield, VA, 1996.
- (12) Innovations in Site Characterization Case Study: Site Cleanup of the Wenatchee Tree Fruit Test Plot Site Using a Dynamic Work Plan; EPA-542-R-00-009; U.S. Environmental Protection Agency, U.S. Government Printing Office: Washington, DC, 2001.

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