

ENVIRONMENTAL DATA ANALYSIS AND STORAGE: DETECTION-LIMIT ISSUES

This letter reports on the recommendations formulated as a policy for handling analytical data from the Rocky Flats Environmental Database System (RFEDS). If acceptable to the Department of Energy (DOE), the policy will provide for consistent treatment of chemical data contained in RFEDS.

There are three related issues:

- (1) How to deal with multiple detection limits
- (2) How to treat non-detects
- (3) How to perform data cleanup

1.0 MULTIPLE DETECTION LIMITS

The standard reporting format for RFEDS data gives one field for the detection limit; unfortunately, this one field contains at least three variables: the instrument detection limit (IDL), the method detection limit (MDL), and the contract-required detection/quantitation limit (CRDL/CRQL). In general, however, this creates a problem only for inorganic analytes (i.e., metals and water-quality parameters).

Examination of detection limits for metals in one data set (containing 1989-93 data), showed an average of nine different detection limits per analyte. Small differences in the IDL over time are expected, and do not generally create a problem for data users. Different analytical methods also have different general detection limits for different analytes (e.g., the MDL for Pb by GFAA may be lower than the general MDL for Pb by ICP). However, the CRDLs for metals (as given in the Environmental Protection Agency's (EPA) Statement of Work (SOW) for Inorganics Analysis) may be one to two *orders of magnitude greater* than the actual IDL. Although this EPA SOW, as referenced in the GRAASP, clearly states that labs should report "*...for each analyte either the value of the result (if the concentration is greater than or equal to the IDL) or the IDL for the analyte corrected for dilutions...*", this requirement has not always been followed. Some laboratories reported the concentration *as* the value of the CRDL if the concentration was above the IDL but below the CRDL. This creates the problem of having non-detect values that are one to two orders of magnitude greater than the values of many detects for that analyte in the same data set. The "Gansecki rule" was proposed (in EPA comments on the *1990 Background Geochemical Characterization Report*) as an attempt to eliminate these high-value non-detects from the data set. The "Gansecki rule" calls for exclusion of all non-detects greater than two times the minimum reporting limit; however, this "rule" has come under criticism as arbitrary and possibly not technically defensible.

1.1 Summary and Recommendations

- Decisions based on a graphical review of the data distribution are thought to be more technically defensible than the general application of an arbitrary rule (i.e. the "Gansecki rule"), even if the "rule" comes from EPA comments. The use of professional judgement and technically arguable reasoning is recommended. It is incumbent upon the data users to document all steps in their analysis of RFEDS data.
- The values of CRDLs for metals, as given in EPA SOW for Inorganics Analysis, should be compared with the data set to ascertain what percentage of the data is reported as the value of the CRDL (see Table 1).

Table 1: INORGANIC TARGET ANALYTE LIST (TAL)

| Analyte | CRDL (ug/L) |
|-----------|-------------|
| Aluminum | 200 |
| Antimony | 60 |
| Arsenic | 10 |
| Barium | 200 |
| Beryllium | 5 |
| Cadmium | 5 |
| Calcium | 5000 |
| Chromium | 10 |
| Cobalt | 50 |
| Copper | 25 |
| Iron | 100 |
| Lead | 3 |
| Magnesium | 5000 |
| Manganese | 15 |
| Mercury | 0.2 |
| Nickel | 40 |
| Potassium | 5000 |
| Selenium | 5 |
| Silver | 10 |
| Sodium | 5000 |
| Thallium | 10 |
| Vanadium | 50 |
| Zinc | 20 |
| Cyanide | 10 |

- The new format for the electronic data deliverable (EDD) proposed by Sample Management will reiterate the need for laboratories to report the actual analytical result in the "concentration field" of the reporting form if that result is greater than the IDL. There will also be a separate field (in addition to the current reporting-limit field) reserved exclusively for the IDL.

2.0 TREATMENT OF NON-DETECTS

As noted in earlier correspondence (August 31, 1993), for those data sets with a high rate of non-detection, the method of replacement affects the value obtained for the mean and upper confidence limit (UCL). However, for as much as 80 percent non-detects, simple substitution and Maximum Likelihood Estimation (MLE) give similar results (see Sanford *et al.*, 1993). In cases with greater than 80 percent non-detects, the results obtained from simple substitution and MLE may be quite different and can lead to different — possibly opposite — conclusions.

Certainly the *worst* possible treatment of non-detects is to drop them from the data set (Helsel, 1990; Sanford *et al.*, 1993). Non-detects should **NEVER** be excluded from any statistical comparison of Operable Unit (OU) versus background data.

Given the cumulative uncertainties throughout the processes of sampling and chemical analysis, the possible error introduced by using simple substitution rather than using MLE replacement of non-detects is probably negligible. The standard practice for treatment of non-detects, as given in EPA statistical guidance, calls for simple substitution using 1/2 the detection limit. However, for RFEDS data, it may be better to use 1/2 the result if the CRDL or the MDL is given in the reporting-limit field instead of the IDL. ←

In the case of severe censoring (>80 percent non-detects), most "...tests have little power to detect differences in central values." (Helsel, 1990). For severely censored data, it may be best to review the spatial and temporal distribution of the detected concentrations for the particular analyte and assess the analyte without using inferential statistics. This common-sense approach would assist in identifying potential sources within the OU and would avoid potentially misleading statistical results. For example, if 81 out of 100 analyses for a given analyte were non-detects, and the remaining 19 detects came from one location within the OU, we have some common-sense useful information. In many ways, this type of spatial and temporal analysis would be akin to that applied for the "hot-measurement" test. ←

The main problem in using inferential statistics for data sets with a high percentage of non-detects is that one ends up comparing the values of different detection limits rather than comparing real data. Because different data sets may have different proportions of the IDL, MDL, or CRDL given in the detection-limit field, using statistical analysis without first looking at the data (via histograms, etc.) may lead to misleading conclusions about the data. The following is a case in point.

Some regulators have questioned the validity of Rocky Flats Plant (RFP) background data, citing those cases where the background mean is statistically significantly *higher* than the OU mean. Other than the percentage expected from the null hypothesis at the 95 percent confidence interval, one reason for a higher background mean (for metals and water-quality parameters) may be that the background and OU data sets have different proportions of data reported as equal to the value of the CRDL (Figure 1a and 1b). The concentration of dissolved barium in groundwater, shown in Figures 1a and 1b, follows a similar distribution for both the OU and background sample populations (ranging from about 10 ppb to about 200 ppb, with a mean around 80 to 90 ppb). There are a few higher values in the OU data (ranging from 210 ppb to 300 ppb), but these account for only about three percent of the total distribution. The obvious difference between Figures 1a and 1b is that 15 percent of the background data were reported as the value of the CRDL (200 ppb), and none of OU data were reported in this manner; hence, the "CRDL syndrome."

The need to visually review the data is critical to any OU versus background comparison. (This need was discussed in Dr. Gilbert's recommendations to EPA, CDH, and DOE, and was included in the "strawman" for determining COCs, presented by EG&G/DOE to the agencies on September 29, 1993). As can be seen in Figures 1a and 1b, a simple histogram tells us more than any list of numbers generated by statistical analysis.

2.2 Summary and Recommendations

- As a replacement value for any non-detect, we recommend the following:
 - Use 1/2 the detection limit, if the IDL is given in the detection-limit field.
 - Use 1/2 the result, if the CRDL is given in the detection-limit field.
- ←

- All data for radionuclides should be used as detects, except for rejected data (validation code = R). For liquid samples, radionuclide data are generally given in units of PCI/L; for solids, radionuclide data are in PCI/G, except for TRITIUM data, which are always in units of PCI/L. Data for which all unit designations are missing should probably be deleted from the working data set.
- For organics, the IDL and the CRQL are similar in magnitude, so the result qualifier or validated result qualifier can generally be used to determine the percentage of non-detects. Many organic analytes are qualified "U" (non-detect), and any "hits" – especially common lab contaminants such as acetone, methylene chloride, and certain phthlates – need to be carefully evaluated. Results from corresponding field blanks or lab blanks should be examined for possible contamination introduced into the samples; these are designated by a "B" in the lab-qualifier field.
- For metals and water-quality parameters, it is ineffective to rely on the result qualifier alone. The following criteria were employed to differentiate detects from non-detects in the *1993 Background Geochemical Characterization Report*, and are suggested as guidelines for all data:

If the qualifier had a "B" code (indicating that the result was above the IDL but below the CRDL), or if the validation code had a "JA" code (estimated value above the IDL but below the CRDL), or if the result was greater than the value in the reporting-limit field, the result was taken to be a detected value. If the observation did not meet at least one of these criteria, then it was taken as a non-detect.

- All data should be reviewed graphically (non-detects and detects together) prior to the application of any statistical tests. This will illustrate any potential problems, such as the "CRDL syndrome."
- For any analyte with a non-detect rate greater than 80 percent, we suggest that the data be evaluated spatially and temporally, using professional judgement. In the case of OU versus background comparisons, this approach will be more informative than the use of inferential statistics.

3.0 ISSUES REGARDING DATA CLEANUP

The so-called "data clean-up" of RFEDS output is mostly a task to make the data consistent. This consists of a time-consuming series of steps (which should be documented by the data user) including the standardization of units, standardization of geologic codes, standardization of locations if the location designation has changed over time, standardization of analyte names (usage has changed over the years), exclusion of quality control data (rinsates, etc.) from the working data set, removal of any rejected (val = 'R') data, replacement of non-validated records with corresponding validated records (if available), correction of incorrect units (e.g., pH should have 'PH' as the unit, *not* 'MG/L' as the unit), averaging of DUP/REAL pairs, appropriate use of DIL data, outlier analysis, et cetera.

The RFEDS has shown continuous improvement in the quality of data contained in the system. Newer data (1992-93) is generally "cleaner" than historic (pre-1992) data. However, all data users need to be made aware of potential pitfalls before applying statistical tests to the data. The steps listed in the previous paragraph give a general overview for the process of data cleanup.

The data clean-up issue was addressed in letter 93-RF-10568, and is part of the Continuous Improvement process for RFEDS and the Sample Management Group.

3.1 Summary and Recommendations

- All data users should carefully document the steps used in the process of data cleanup. If questions arise, review of this documentation should be able to provide the necessary information.
- RFEDS and the Sample Management Group are committed to Continuous Improvement; recent data (1992 to present) have fewer problems than historic data (pre-1992). Issues of duplicate records, incorrect units, etc., are currently being addressed.