

Treatment of analytical results below the Detection Limit in DIVER Explorer

When laboratories analyze samples, they report a detection limit, the concentration below which they cannot reliably report the concentration. (In addition, there may also be a reporting limit, which specifies a concentration range above the detection limit with greater uncertainty as to quantitation of the concentration.) When analyzing the data, the user must make decisions on how to include these non-detect values, particularly when summing concentrations and when looking at statistical differences between samples. Ideally, the number of non-detect values is relatively low and the user has sufficient knowledge about the distribution of the contaminant data to make statistical estimations of non-detect values (e.g., see Helsel, 2005, "More Than Obvious: Better Methods for Interpreting Nondetect Data" at <http://pubs.acs.org/doi/pdf/10.1021/es053368a> for a publicly available review of the process). EPA Region III has an additional resource explaining how different quantitation and detection limits are calculated in the laboratory. This is available at <https://www.epa.gov/quality/idl-mdl-pql-what-l-going-what-does-all-alphabet-soup-really-mean>.

However, as a basic screening-level approach, Explorer provides three basic options for values to assign to the non-detected analytes: 0, $\frac{1}{2}$ and 1 times the appropriate detection limit. From a screening standpoint, using zero provides a minimum bound on contaminant concentration, while substituting the full detection limit provides the upper bound. Substitution of $\frac{1}{2}$ the detection limit is a common "middle-of-the-road" approach for approximations.

Additionally, when reporting multiple contaminants, Explorer provides the option of assigning values of $-\frac{1}{2}$ and -1 times the detection limit. Because of the condensed tabular structure of the multiple contaminant outputs (concentrations of multiple contaminants listed in columns, with each sample only assigned one row), qualifiers and detection limits for individual analytes are not reported. Substituting negative values for the non-detects allows the user to quickly assess the extent of non-detects in their data set for each contaminant, as well as what those detection limits are.