The USEPA has issued several comprehensive documents dealing with calculating upper limits to compute BTV estimates ((USEPA 2002), (USEPA 2002), (USEPA 2006), (USEPA 2009), (USEPA 2015)) based upon a background dataset. However, there is no general consensus among practitioners about the statistic (upper limits) that should be used to estimate a BTV. For the sake of a typical reader and completeness, a brief description of upper limits (with interpretation), including upper percentiles, UPLs, UTLs, and USLs, used to estimate BTVs is provided in this appendix. Mathematical details and formulae to compute these statistics for datasets with and without NDs are given in ProUCL 5.1 Technical Guide. In the following the background population is also referred as the target population.

Upper percentile: A value, based on the data, below which a selected percentage (for example, 95%) of the data points will fall. In comparison with other BTV estimates (for example, UTL 95-95), the use of the 95th percentile yields a higher number of false positives, resulting in potentially unnecessary cleanup decisions, especially when many observations coming from a population (comparable to the background population) are compared with the sample percentile, p0.95.

Upper prediction limits (UPL): Let UPL95 represent a 95% UPL for a future/next observation. One is 95% sure that a *single* future value from the target (background) population will be less than or equal to the UPL95 with a confidence coefficient of 0.95 (95%). If an on-site value, x_onsite, is less than the UPL95, it may be concluded that x_onsite comes from the background population with a CC of 0.95. A UPL95 is not meant to be used to perform more than one future comparison.

However, in practice, users tend to use a UPL95 for many future comparisons, which results in a higher number of false positives (locations declared contaminated when in fact they are clean). When k (>1) future comparisons are made with a UPL95, some of those values will exceed UPL95 just by chance, each with a probability of 0.05. For proper comparison, UPLs need to be computed according to the number, k, of comparisons that will be performed. For details refer to ProUCL 5.1 Technical Guide.

Upper tolerance limit (UTL): A UTL (1-α)-p (for example, UTL 95-95) based upon an established background dataset represents that limit such that p% (for example, = 95%) of the sampled data will be less than or equal to that limit with a CC equal to (1-α) * 100% (for example, =95%). A UTL (1-α)-p represents a (1–α) * 100% upper confidence limit for the p^{th} percentile of the underlying background population. It is expected that at least p% of the observations coming from the background population will be less than or equal to the UTL (1-α)-p with a CC equal to (1-α) * 100%. Specifically, a UTL 95-90 represents an upper tolerance limit providing coverage to at least 90% of the observations of the target population with CC=95%.

A UTL 95-90 assumes that as much as 10% of the observations can exceed the background UTL 95-90 when site concentrations are not different from the background population, and a UTL 95-90 can declare 10% of the observations coming from the background population as not coming from the background population just by chance, with a probability of 0.95. A UTL is used when many comparisons are planned. For a UTL 95-90, 10 exceedances per 100 comparisons (of background values) can result just by chance for an overall CC of 0.95. The number (and not percentage) of false positives can become large when many values from the target population are compared with a UTL.

Upper simultaneous limit (USL): A (1 – α) * 100% USL based upon an established background dataset is meant to provide simultaneous coverage for all sample observations in the background dataset (Singh and Nocerino, 1995) with probability (1-α). It is expected that all observations (present and future) belonging to the target (background, comparable to background) population will be less than or equal to a 95% USL (USL95) with a CC=0.95.

Like a UTL, a USL is used when any number (small or large) of on-site observations are compared with a BTV estimate. Unlike a UTL, a USL does not assume a priori that a certain percentage of background observations may not belong to the background population. Depending upon the variability of the background data, some of these statistics (for example, USL95, UTL 95-95) may exceed the largest value in the background dataset. To account for data variability of all sampled and unsampled locations, critical values associated with a USL95 increase as the sample size increases.