

Evaluation of UCL-Related DQOs

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The Data Quality Objectives (DQOs) for human health and ecological risk assessment address data adequacy for calculating the UCL. Evaluated in this section, the UCL-related DQO recognizes the importance of obtaining exposure point concentrations (EPC) that address uncertainty in a conservative manner (controlled by alpha-type error rate), but at the same time are not “too conservative” (controlled by beta-type error rate). In risk terminology, alpha pertains to error rate of “false determination of acceptable”, while the beta pertains to the error rate of “false determination of exceedance”.

In risk assessment, alpha is theoretically presumed to be met by the use of a 95% UCL to estimate EPC, regardless of sample size. For the 95% UCL to meet its stated alpha of 0.05, random sampling assumptions must be valid. An additional assumption often required for analytical concentration results is that “below detection” data must be either handled either accurately or conservatively. In contrast, a beta-type error rate of 20% may not always be met and may actually be impossible to meet without compromising alpha. Therefore to evaluate DQOs related to the UCL (or more generally, the EPC), alpha (conservatism) is assumed fixed at 0.05 and only beta-type error, or accuracy (not “too conservative”), is evaluated. An implication of evaluating beta (and sample size in general), is that cases are highlighted where the risk decision (“exceedance”) is likely to be overly conservative and additional samples may be beneficial in reducing estimated risk.

Although the concepts of “false acceptance” or “false exceedance”, are applicable to other study areas, quantitative assessment of alpha and beta require the assumption that all samples are independent random samples of the same population. Therefore, DQO’s are only evaluated in detail for study areas where random sampling was applied, namely RCRA Canyon, Remaining Onsite area, and Former Ponds and Pads.

The statistical methodology and key statistical definitions are presented below followed by the evaluation of UCL-Related DQOs for each of three study areas listed above.

STATISTICAL METHODOLOGY

Accuracy or Power to Discriminate

When estimating a parameter such as the mean or UCL, the probability $1 - \beta$ has the interpretation of “power to discriminate” the mean relative to *any* selected constant of interest, i.e. the accuracy of estimating the mean. Thus the DQO of meeting beta equal to 20% is statistically ambiguous since a selected constant was not also stated. In fact, a single constant, with which to assess sample size and accuracy for EPC estimation, is not suggested or promoted in risk-related or DQO-related guidance documents even though power and sample size are important considerations in assessing uncertainty. The inclusion of beta in a DQO statement allows power and sample size to be evaluated within the site-specific decision structure relevant to the risk assessment.

Accuracy relative to a selected constant is directly related to post-sampling power when alpha is fixed. For risk assessment, accuracy can be evaluated relative to two distinct constants:

- “Estimation Accuracy” is defined as accuracy relative to the population mean; and
- “Decision Accuracy” is defined as accuracy relative to the risk screening level(s).

Both types of accuracy, or conversely uncertainty, are relevant to risk assessment. Estimation uncertainty directly relates to sample size and informs us whether additional sampling would be effective. However decision uncertainty informs us whether additional sampling is necessary. Even with high estimation uncertainty, if the estimation uncertainty does not impact the risk decision, then sample size and power are be “good enough”. For example, often cases with high estimation uncertainty have very low frequencies of detection, and yet these same cases may be of least concern in the risk assessment (i.e. they have low decision uncertainty).

Estimation and decision uncertainty are defined quantitatively below with calculations presented in Tables B4 – 1 through B4 – 3.

Estimation Uncertainty as Relative Estimation Interval

A simple measure of estimation accuracy for the EPC (whether UCL or maximum detection) is the distance between the EPC and the population mean as estimated by the *sample mean*. The sample mean is used as a surrogate for the population mean because, given our current data, it is the most likely point estimate for the true population mean

- Estimation interval = (EPC – sample mean); and
- Relative estimation interval = (EPC – sample mean)/sample mean.

Because contaminant distributions are typically skewed and have the theoretical property that the variance increases relative to the mean (e.g. lognormal distribution), the estimation interval is most comparable between cases when it is re-scaled by dividing by the sample mean. The resulting “relative estimation interval” (REI) is the estimation interval stated as a percentage of the mean. Estimation accuracy is considered adequate if the REI is less than or equal to 100% of the sample mean.

Decision Uncertainty

For the purposes of this DQO evaluation, the “risk decision” is simplified to comparison of the EPC to a single criterion that considers ecological and human health risk, and also the background UTL in cases where background levels are present and characterized (metals and dioxins). This single screening level (SL) is defined as the lowest toxicological screening level, or, when considering background, the maximum of (i) the lowest toxicological screening level and (ii) the UTL of background.

Uncertainty in the risk decision is said to be low, if the entire estimation interval, i.e. *both* the point estimate (mean) and the upper bound estimate (UCL or max), is below the SL. Likewise decision uncertainty is said to be low if the entire estimation interval is above the SL. The only case where decision accuracy is compromised is when the estimation interval spans the SL, with the mean lower and the EPC higher.

Evaluation of DQOs Using Estimation and Decision Uncertainty

The evaluation rule considering both types of uncertainty is relatively simple:

Cases are considered to adequately meet UCL-related DQOs if either or both estimation uncertainty or decision uncertainty is low.

A re-statement of this rule is that cases are considered to inadequately meet DQOs only when both estimation and decision uncertainty are high.

The rationale for concluding the DQO to be met even if only one type of accuracy is adequate is as follows.

If estimation uncertainty is high (i.e. REI > 100%) yet decision uncertainty low (mean and EPC are *both below* the SL or *both above* the SL), then the DQO is adequately met because the estimation uncertainty, regardless of how high, does not impact the decision.

Alternatively, if decision uncertainty is high (i.e. the estimation interval spans the SL) and estimation uncertainty is low, then additional sample data provide little benefit and the DQO is adequately met. This case arises when the true population mean is very close to the SL. In this case, even estimation accuracy that is adequate from a sampling efficiency view-point, might still not be tight enough to avoid a “false exceedance”. When the population and/or sample mean is near to and less than the SL, a large beta-type error (probability of “false exceedance”) is unavoidable under any feasible amount of sampling. Formally stated, the beta-type error cannot be reduced further without compromising the alpha-type error (reducing confidence).

In short, it is only in cases where decision uncertainty is high and estimation uncertainty is high that the beta-type error can be reduced (with additional sampling) while at the same time maintaining alpha at 0.05.

UCL-RELATED DQO EVALUATION

Compounds which do not meet the UCL-Related DQOs, as stated above, are identified with underline below for each study area. Additional detail about these cases as well as example cases which do meet DQOs is also provided.

RCRA Canyon

Metals

Decision uncertainty is adequately low for all metals with the exception of copper and manganese. Estimation uncertainty for copper is adequately low while estimation uncertainty for manganese is slightly elevated. Therefore, EPC-Related DQOs are considered approximately met for copper, and adequately met for all other metals.

PCB and Dioxins

Decision uncertainty is adequately low for all PCB and dioxin compounds shown in Table B4-1, with the possible exception of Avian PCB Congener toxic equivalency quotient (PCBC TEQ), for which an SL was not available. With estimation uncertainty moderate for this compound, the DQO may not be met for Avian PCBC TEQ. The DQO is met for the remaining PCB and dioxin compounds.

Pesticides

Decision uncertainty is adequately low for all pesticide compounds shown in Table B4-1. Therefore the DQO is met for all pesticide compounds.

PAH and SVOC

Decision uncertainty is adequately low for all polycyclic aromatic hydrocarbons (PAH) and semi-volatile organic compounds (SVOCs) shown in Table B4-1, with the possible exception of benzo(g,h,i)perylene for which an SL was not available. Since estimation uncertainty is adequately low for benzo(g,h,i)perylene, the DQO is met for all PAH and SVOC compounds.

Many compounds had moderate to high estimation uncertainty above 100% (REIs of 199% to 3498%) however higher REIs are generally associated with frequencies of detection at or below 6%. Again this high estimation uncertainty is due to the low rate of detection causing maximum detected concentrations or other conservative methods to be used for the EPCs. However, since the estimation intervals for these compounds are well below the SLs, the decision uncertainty is not impacted.

VOCs

Decision uncertainty is adequately low for all VOC compounds shown in Table B4-1, with the possible exception of 1,2-dichloroethene and propanal, for which SLs were not available. With estimation uncertainty high for these two compounds, the DQO may not be met for 1,2-dichloroethene and propanal. However, DQOs are met for the remaining VOC compounds.

Estimation uncertainty is high for many VOC compounds (REIs of 319% - 822%), particularly in cases where frequency of detection is at or lower than 10%, again due to use of maximum detected concentrations or other conservative methods for the EPCs. However, since the estimation intervals for these compounds are well below the SLs, the DQOs are met.

Remaining Onsite Area

Cyanide

Decision uncertainty is adequately low for total cyanides as is estimation uncertainty. Therefore the DQO is well met for cyanide.

Metals

Decision uncertainty is adequately low for all metals, with the exception of lead. For lead, the estimation uncertainty is calculated as being negative due to an inconsistency in the data sets used for calculating the mean and for calculating the UCL. On a given data set, the UCL should always be higher than the mean, and therefore a negative value for REI would be impossible (aside from severe non-detect handling artifacts which are not the case for this metal). Therefore, the REI is not currently accurate and the DQO may not be met for lead. However, the DQO is well met for all other metals.

PCB and Dioxins

Decision uncertainty is adequately low for all PCB and dioxin compounds in Table B4-2, with the exception of mammalian PCBC TEQ, and possibly avian PCBC TEQ (for which an SL was not available). With estimation uncertainty for these two compounds also high, the DQO is not met for mammalian PCBC TEQ and may not be met for avian PCBC TEQ. However the DQO is met for the remaining PCB and dioxin compounds.

Since mammalian PCBC TEQ has a mean of 4.4 mg/kg and EPC of 16.4 mg/kg (the maximum detected concentration), the large estimation interval spans the SL of 15.92 mg/kg. Therefore estimation uncertainty for this compound impacts the risk decision and implies a much larger probability than desired for the beta-type error ("false exceedance"). Furthermore, additional sampling is likely to reduce estimation uncertainty to the degree that decision uncertainty can be eliminated. Restated, the probability of a beta-type error ("false exceedance") is much larger than desired for mammalian PCBC TEQ and additional sampling would likely help to bring the EPC for this compound below the SL.

Herbicides and Pesticides

Decision uncertainty is adequately low for all herbicide and pesticide compounds shown in Table B4-2, as is estimation uncertainty. Therefore DQOs are well met for all herbicides and pesticides.

PPO

Decision uncertainty is adequately low for tert-butyl alcohol (TBA), as is estimation uncertainty. Therefore the DQO is well met for TBA.

PAH and SVOC

Decision uncertainty is adequately low for all PAH and SVOC compounds shown in Table B4-2, with the exception of n-nitrosopyrrolidine and possibly benzo(g,h,i)perylene (for which an SL was not available). For n-nitrosopyrrolidine, the estimation uncertainty is calculated as being negative due to an inconsistency in the data sets used for calculating the mean and for calculating the UCL. Therefore, the REI is not currently accurate and the DQO may not be met for n-nitrosopyrrolidine. With estimation uncertainty adequately low for benzo(g,h,i)perylene, the DQO is met for all PAH and SVOC compounds, with the exception of n-nitrosopyrrolidine.

VOCs

Decision uncertainty is adequately low for all VOC compounds shown in Table B4-2, except possibly for isopropanal and propanal, for which SLs were not available. With estimation uncertainty for these compounds also high, the DQO may not be met for isopropanal, and propanal. The DQO is met for the remaining VOCs.

Former Ponds and Pads

Metals

Decision uncertainty is adequately low for all metals with the exception of barium. With estimation uncertainty moderately elevated the DQO is not met for barium. However the DQOs are met for the remaining metals.

The sample mean of barium is somewhat close to the SL and 4 outliers are approximately 10 times the SL. Therefore, although additional samples might bring the EPC estimate closer to the sample mean, this may effect my not be strong enough to reduce estimation error to the extent that it would cause the barium EPC to be below the SL.

PCB and Dioxins

Decision uncertainty is adequately low for all PCB and dioxin compounds in Table B4-3, with the exception of Sum of PCB Congeners and possibly Avian PCBC TEQ, for which an SL was unavailable. With estimation uncertainty moderately high for these two compounds the DQO is not met for Sum of PCB congeners and may not be met for Avian PCBC TEQ. The DQO is met for the remaining PCB and dioxin compounds.

Both congener summation terms, for Avian TEQ and for total PCB are highly skewed, apparently due to relatively large detections and associated high detection limits. Therefore, reduction of estimation uncertainty enough to bring the UCL closer to the mean and below the SL for sum of congeners, thereby meeting the DQO, would likely require a large number of additional PCB congener samples.

Herbicides and Pesticides

Decision uncertainty is adequately low for all herbicide and pesticide compounds shown in Table B4-3. Therefore the DQO is met for all herbicides and pesticides

PPO

Decision uncertainty is adequately low for acrolein and tert-butyl alcohol (TBA) as is estimation uncertainty. Therefore the DQO is well met for both compounds.

PAH and SVOC

Decision uncertainty is adequately low for all PAH and SVOC compounds shown in Table B4-3, with the exception of n-nitrosodimethylamine, and possibly benzo(g,h,i)perylene, for which an SL was not available. The estimation uncertainty for both analytes is calculated as being negative due to an inconsistency in the data sets used for calculating the means and UCLs. Therefore, the REIs are not currently accurate and the DQO may not be met for n-nitrosopyrrolidine and benzo(g,h,i)perylene. However, the DQO is adequately met for the remaining PAH and SVOC compounds.

VOCs

Decision uncertainty is adequately low for all VOC compounds shown in Table B4-3, with the possible exceptions of 1,2-dichloroethene, isopropanal, and propanal, for which SLs were not available. The estimation uncertainty for all three compounds is calculated as being zero or negative due to an inconsistency in the data sets used for calculating the means and UCLs. Therefore, the REIs are not currently accurate and the DQO may not be met for 1,2-dichloroethene, isopropanal, and propanal. The DQO is met for the remaining VOCs.