|  |  |
| --- | --- |
|  | Annex 5  Ref. §3.7 |
| OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic | |
| Meeting of the Working Group on Monitoring and on Trends and Effects of Substances in the Marine Environment (MIME)  Copenhagen: 19–23 November 2018 | |

Reporting of less-than values and uncertainties for chemical concentrations

This Annex aims to clarify the way that less-than values and uncertainties should be reported to the ICES database. It applies to the reporting of chemical concentration measurements (and biological effects measurements, such as bile metabolite concentrations or EROD activities, which must be positive and which have limits of detection and quantification analogous to those for concentration measurements). Correct reporting of less-than values and uncertainties is important to avoid spurious results in the OSPAR MIME assessment.

# Recommended way of reporting less-than values

Chemical measurements can be reported to the ICES database as either the measured value or as a less‑than value. The limit of detection should be used to determine whether the measured value or a less-than value is reported, with measured values below the limit of detection being reported as less-than values. (In practice the limit of quantification is sometimes used, although this is not recommended – see later.) If a measurement is reported as a less-than value, then a data-analyst should subsequently infer that that the measured value is somewhere between zero and the reported value. For example, a less-than value of 0.3 should mean that the measured value is somewhere between 0 and 0.3.

Let:

* MV be the measured value for a sample;
* LOD be the limit of detection for the sample
* LOQ be the limit of quantification for the sample

The reporting of these data involves four variables:

* VALUE is a number that gives either the measured value or a less-than value
* [QFLAG](https://vocab.ices.dk/?ref=180) is a code that indicates whether VALUE is the measured value or a less-than value and, in the latter case, describes whether the less-than value is based on the limit of detection or quantification
* [DETLI](https://vocab.ices.dk/?CodeID=54316) is a number that gives the limit of detection
* [LMQNT](https://vocab.ices.dk/?CodeID=54317) is a number that gives the limit of quantification

The data should be reported as:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case | VALUE | QFLAG | DETLI | LMQNT |
| LOQ < MV | MV |  | LOD | LOQ |
| LOD < MV ≤ LOQ | MV |  | LOD | LOQ |
| MV ≤ LOD | LOD | D | LOD | LOQ |

Notes:

* There is redundancy in these reporting rules in that QFLAG can be inferred from VALUE and DETLI. However, the redundancy is useful for trapping reporting errors. Also, all four variables (VALUE, QFLAG, DETLI and LMQNT) are required for the alternative ways of reporting that are sometimes used (see later).
* QLAG is not intended to identify measured values that are between the LOD and the LOQ. Data-analysts who require this information should infer it from VALUE and LMQNT.
* A common practice in statistical analyses is to replace less-than values by half the limit of detection (or some similar calculation). Measured values below the LOD should always be reported with VALUE = LOD; i.e. never report VALUE = LOD /2 (or similar).

# Alternative acceptable ways of reporting less-than values

Sometimes it is not possible to follow the recommended approach for reporting less-than values described above. This can arise e.g. because the analytical laboratory has not provided the reporting institute with the required information, or because there are limitations in the database operated by the reporting institute. Different scenarios are listed below with guidelines on how the data should be reported.

1. The MV and the LOD are available but the LOQ is not:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case | VALUE | QFLAG | DETLI | LMQNT |
| LOD < MV | MV |  | LOD |  |
| MV ≤ LOD | LOD | D | LOD |  |

1. The MV is only available when above the LOQ:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case | VALUE | QFLAG | DETLI | LMQNT |
| LOQ < MV | MV |  | LOD | LOQ |
| MV ≤ LOQ | LOQ | Q | LOD | LOQ |

Notes:

* Some analytical laboratories only provide measured values above the LOQ, arguing that measured values below the LOQ have greater uncertainty. However, this results in a loss of information (compared to the recommended way of reporting) when the measured value is between the LOD and LOQ. The increase in uncertainty can be accounted for in the statistical analysis of the data, provided that the uncertainty associated with the measured value is correctly reported (see later in this document).
* If the analytical laboratory provides measured values below the LOD as <LOD and measured values between the LOD and LOQ as <LOQ, then QFLAG = Q and VALUE = LOQ should be used in both cases. A mixture of QFLAG = Q and QFLAG = D should be avoided because it introduces bias into the statistical assessment. The problem is that, when QFLAG = Q, the data-analyst will infer that the measured value is between 0 and LOQ, whereas it is actually between LOD and LOQ.
* If the LOD is not available, DETLI should be left blank.

1. The LOD and LOQ are available but cannot be reported in DETLI and LMQNT:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case | VALUE | QFLAG | DETLI | LMQNT |
| LOQ < MV | MV |  |  |  |
| LOD < MV ≤ LOQ | MV |  |  |  |
| MV ≤ LOD | LOD | < |  |  |

Note: this situation might appear unlikely, but there are situations where e.g. the LOD is greater than the accredited limit of detection of an analytical laboratory, but only the accredited limit of detection can be passed on to a third party. This might arise when e.g. the volume of sample material for chemical analysis is smaller than typically analysed.

1. Data are available with less-than values indicated by the “<” prefix, but it is unclear whether these refer to the LOD or LOQ:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case | VALUE | QFLAG | DETLI | LMQNT |
| MV | MV |  |  |  |
| Less-than value | Less-than value | < |  |  |

# DATSU checks on less-than values beginning in June2019

DATSU is the data screening programme that checks data submissions for errors and inconsistencies. The reporting institute will receive the following warning / error messages if the data are incorrectly reported.

|  |  |  |  |
| --- | --- | --- | --- |
| Check | MYEAR ≥ 2019 | MYEAR = 2018 | MYEAR < 2018 (legacy data) |
| Multiple QFLAG values | Critical error | Critical error | Error |
| VALUE ≠ DETLI and QFLAG = D | Critical error | Critical error | Error |
| VALUE ≠ LMQNT and QFLAG = Q | Critical error | Critical error | Error |
| LMQNT < DETLI | Critical error | Critical error | Error |
| VALUE ≤ DETLI and QFLAG = NULL | Error | Warning | Warning |
| VALUE ≠ DETLI and QFLAG = < | Error | Warning | Warning |
| VALUE = DETLI and QFLAG = < | Warning | Warning |  |
| QFLAG = < and LMQNT ≠ NULL | Warning | Warning |  |

# Uncertainties

The reporting of uncertainties involves two variables:

* [UNCRT](https://vocab.ices.dk/?CodeID=54314) is a number giving the analytical uncertainty in the measurement reported in VALUE
* [METCU](https://vocab.ices.dk/?ref=213) is a code that describes the method for expressing uncertainty

UNCRT only relates to analytical uncertainty and does not include any aspects of sampling uncertainty. UNCRT should ideally include all aspects that contribute to the analytical uncertainty in the measurement reported in VALUE. However, for MIME assessment purposes, it is acceptable if UNCRT only includes the most important aspects contributing to the analytical uncertainty; i.e. reporting institutes do not need to take any measures if some minor aspects (e.g. dilution effects) are not included in the uncertainty calculations they are provided with.

The uncertainty calculation should include a relative component and a constant component. The relative component will dominate when the measured value is above the LOQ. The constant component will have an increasing effect as the measured value decreases below the LOQ and will dominate when the measured value is close to the LOD. Analytical laboratories often provide uncertainties based only on the relative component, even when the measured value is below the LOQ. However, this approach makes the uncertainty of values below the LOQ too small and consequently these observations will have too much influence on the statistical analysis of the data in the MIME assessment.

A simple way of calculating an uncertainty that includes the constant component is as follows. Suppose that the analytical laboratory provides uncertainties based only on only relative component *v*. Thus the uncertainties received from the analytical laboratory would be 100 × *v* (if provided as a percentage) or VALUE × *v* (if provided as a standard deviation) or 2 × VALUE × *v* (if provided as an expanded uncertainty). Let *s* be the standard deviation of the replicate measurements of the blank used to define the LOD (for example, the LOD might typically be defined as 3 × *s*). Then let



The uncertainty incorporating both the relative and constant components is then:

UNCRT = *u* if expressed as a standard deviation (METCU = SD)

UNCRT = 2 × *u* if expressed as an expanded uncertainty (METCU = U2)

UNCRT = 100 × *u* / VALUE if expressed as a percentage (METCU = %)

Uncertainties should be reported with METCU = U2 or SD. Using METCU = % will result in a warning (with a critical error if VALUE = 0).

UNCRT should always be ≥ 0.