

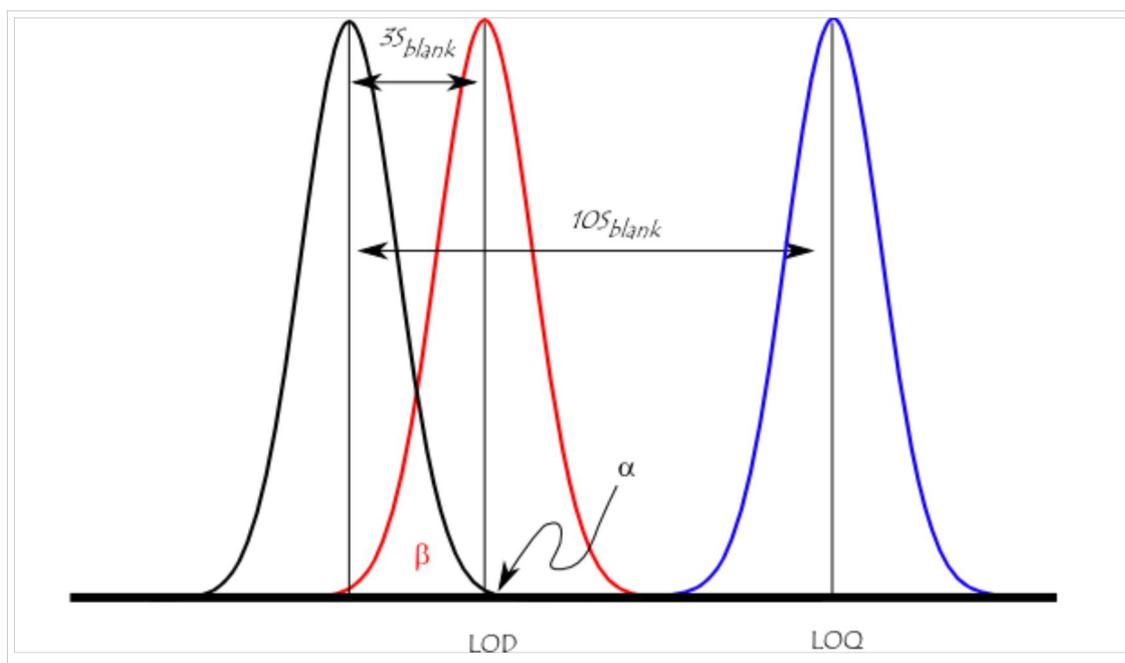
Detection limit

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In analytical chemistry, the **detection limit**, **lower limit of detection**, or **LOD** (limit of detection), is the lowest quantity of a substance that can be distinguished from the absence of that substance (a *blank value*) within a stated confidence limit (generally 1%).^{[1][2]} The detection limit is estimated from the mean of the blank, the standard deviation of the blank and some confidence factor. Another consideration that affects the detection limit is the accuracy of the model used to predict concentration from the raw analytical signal.

There are a number of different "detection limits" that are commonly used. These include the **instrument detection limit (IDL)**, the **method detection limit (MDL)** and the **limit of quantitation (LOQ)**. Even when the same terminology is used, there can be differences in the LOD according to nuances of what definition is used and what type of noise contributes to the measurement and calibration.^[3]

The figure illustrates the relationship between the blank, the limit of detection (LOD), and the limit of quantification (LOQ) by showing the probability density function for normally distributed measurements at the blank, at the LOD defined as 3 * standard deviation of the blank, and at the LOQ defined as 10 * standard deviation of the blank. For a signal at the LOD, the alpha error (probability of false positive) is small (1%). However, the beta error (probability of a false negative) is 50% for a sample that has a concentration at the LOD (red line). This means a sample could contain an impurity at the LOD, but there is a 50% chance that a measurement would give a result less than the LOD. At the LOQ (blue line), there is minimal chance of a false negative.



Contents

- 1 Instrument detection limit
- 2 Method detection limit
- 3 Limit of quantification
- 4 Example
- 5 References
- 6 External links

Instrument detection limit

Most analytical instruments produce a signal even when a blank (matrix without analyte) is analyzed. This signal is referred to as the noise level. The IDL is the analyte concentration that is required to produce a signal greater than three times the standard deviation of the noise level. This may be practically measured by analyzing 8 or more standards at the estimated IDL then calculating the standard deviation from the measured concentrations of those standards.

Method detection limit

Many times there is more to the analytical method than just doing a reaction or submitting it to direct analysis. For example it might be necessary to heat a sample that is to be analyzed for a particular metal with the addition of acid first (this is called **digestion**). The sample may also be diluted or concentrated prior to analysis on an instrument. Additional steps in an analysis add additional opportunities for error. Since detection limits are defined in terms of error, this will naturally increase the measured detection limit. This detection limit (with all steps of the analysis included) is called the MDL. The practical method for determining the MDL is to analyze 7 samples of concentration near the expected limit of detection. The standard deviation is then determined. The one-sided t distribution is determined and multiplied versus the determined standard deviation. For seven samples (with six degrees of freedom) the t value for a 99% confidence interval is 3.14. Rather than performing the complete analysis of seven identical samples, if the Instrument Detection Limit is known, the MDL may be estimated by multiplying the Instrument Detection Limit or Lower Level of Detection by the dilution prior to analyzing the sample solution on the instrument. This estimation, however, ignores any uncertainty that arises from performing the sample preparation and will therefore probably underestimate the true MDL.

Limit of quantification

Just because we can tell something from noise does not mean that we can necessarily know how much of the material there actually is. The LOQ is the limit at which we can reasonably tell the difference between two different values. The LOQ is drastically different between labs so another detection limit is commonly used that is referred to as the **Practical Quantitation Limit** (PQL). The PQL is defined simply as about 5 times the MDL.

Example

It is often difficult to understand the concept of detection limit. The following example may help to clarify some of the concepts defined above.

Suppose you are at an airport with lots of noise from jets taking off. If the person next to you speaks softly, you will probably not hear them. Their voice is less than the LOD. If they speak a bit louder, you may hear them but it is not possible to be certain of what they are saying and there is still a good chance you may not hear them. Their voice is $>LOD$ but $<LOQ$. If they speak even louder, then you can understand them and take action on what they are saying and there is little chance you will not hear them. Their voice is then $>LOD$ and $>LOQ$. Likewise, their voice may stay at the same loudness, but the noise from jets may be reduced allowing their voice to become $>LOD$. Detection limits are dependent on both the signal intensity (voice) and the noise (jet noise).

References

- [^] International Union of Pure and Applied Chemistry. "detection limit (<http://goldbook.iupac.org/L03540.html>) ". *Compendium of Chemical Terminology* Internet edition.
- [^] "Guidelines for Data Acquisition and Data Quality Evaluation in Environmental Chemistry", *Anal. Chem.* **52**: 2242–49, 1980
- [^] Long, Gary L.; Winefordner, J. D. (1983), *Anal. Chem.* **55** (7): 713A–724A

External links

- Downloads of articles (a.o. harmonization of concepts by ISO and IUPAC) and an extensive list of references (<http://www.chemometry.com/Research/LOD.html>)

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