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NATIONAL WATER QUALITY LABORATORY TECHNICAL MEMORANDUM 1996.12

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From: Peter F. Rogerson, Chief
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Subject: Change in the calculation of values for inorganic carbon, total in bottom material

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Revision: None

SCOPE

When the National Water Quality Laboratory (NWQL) changed its computer program for calculating concentrations of inorganic carbon in sediment, we discovered that the old computer program was calculating the results incorrectly. A study, designed to estimate the magnitude of the error, demonstrated that the incorrectly calculated results were about 3 percent higher than the correctly calculated results. Although we cannot accurately establish the length of time that the incorrect calculation was used, we know that the length is at least 10 years or longer.

The NWQL will implement the correct calculation beginning October 1, 1996.

BACKGROUND

The approved method for determining inorganic carbon in bottom material is published in Techniques of Water-Resources Investigations of the United States Geological Survey, Book 5, Chapter A3, "Methods for the Determination of Organic Substances in Water and Fluvial Sediments" by Wershaw and others (1987). The method number for analysis is 0-5102-83.

The computer system which was used to calculate the results for this analysis was retired, and a new computer system was programmed. After this change, we discovered that the original computer program was incorrectly calculating the results for inorganic carbon in bottom material samples.

The error in inorganic carbon will also affect the results for organic carbon in bottom material as inorganic carbon is subtracted from total carbon to obtain organic carbon.

As part of our normal operating procedure, the NWQL analyzes every tenth sample in duplicate. The data from all the duplicate samples analyzed over the last year (30 pairs of samples) were used not only to evaluate the magnitude of the error but also to describe the precision between duplicate samples for the inorganic carbon analysis. This allowed the error to be compared to the analytical precision of the method in an effort to evaluate the impact on the data base. The concentration in the samples ranged from 0.6 to 54 grams per kilogram (g/kg) which represents fairly well the range of values typically encountered for this analysis.

To evaluate the magnitude of the error, the incorrectly calculated results were recalculated correctly. The ratio of the correct results to the incorrect result was calculated and expressed as a percentage.

Duplicate precision was expressed as the ratio of the two analyses (as a percentage), and the mean and standard deviation of ratios was calculated.

DISCUSSION AND CONCLUSIONS

Although the magnitude of the error was a function of the barometric pressure on the day of analysis, we concluded that the incorrect results were approximately 3 percent higher than the correct results over the range of barometric pressures experienced during the year.

The average agreement between duplicate samples (precision) is 98 percent and the standard deviation (relative error) is about 8 percent.

The NWQL will start reporting the correct concentrations beginning October 1, 1996.

For reported concentrations less than 10 g/kg, this change will result in lowering concentrations up to 0.3 g/kg. For reported concentrations between 10 and 100 g/kg, this change will result in lowering values up to 3 g/kg. In many cases, concentrations will be unaffected because of rounding.

Organic carbon in bottom material is obtained by subtracting inorganic carbon from total carbon. The new calculations for inorganic carbon will affect concentrations reported for organic carbon in bottom material. In all cases, organic carbon concentrations obtained by subtraction will be either unaffected or slightly higher. Since the ratio of total carbon to inorganic carbon varies from sample to sample, the difference in organic concentrations must be individually determined.

Impact on the Data Base:

Reported values for inorganic carbon in bottom material will be approximately 3 percent lower than reported in the past. Concentrations for organic carbon in bottom material (obtained by subtraction of inorganic carbon from total carbon) may be slightly higher.

As the magnitude of the error is less than the duplicate precision of the analysis, the change may not be apparent in small data sets. However, the change may be apparent in data sets containing a large number of replicate samples. The change may also be discernible in trend analyses.

The NWQL will not retroactively correct the values in the data base. However, data users should review their data sets and evaluate the impact of the change.

Supersedes: None

Key words: carbon, inorganic, bottom material, calculation, change

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