



Uncertainty Assessment of Copper Content in Water by Atomic Absorption Spectrophotometry

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Abstract

Taking the soluble copper content in water quality samples as the research object, a mathematical model was established and flame atomic absorption spectrophotometry was used to analyze the uncertainty components that affect the measurement results, including the standard solution, standard curve, sample repeatability, sampling volume, and experimental instruments used in the standard. The experimental results indicate that the copper content in the water quality sample is (1.53 ± 0.060) mg/L, and the sampling volume and standard curve measurement are the main sources of uncertainty. Optimizing the use of measuring instruments in experiments and improving the operational skills of operators can effectively reduce uncertainty and improve measurement accuracy.

Subject Areas

Environmental Protection

Keywords

Atomic Absorption Spectrophotometry, Water Quality Monitoring and Analysis, Uncertainty, Mathematical Model, Influence Factor

1. Introduction

With the acceleration of industrialization and urbanization, especially water pollution, heavy metal pollution has become a global environmental problem. Industrial wastewater (such as mining, smelting, electroplating, etc.), agricultural emissions (pesticides, fertilizers), domestic sewage, and atmospheric deposition are all

the main sources of heavy metal pollution in current water quality. Heavy metal pollution not only exists in local areas, but has gradually spread to rivers, lakes, groundwater, and even oceans, with a wide range of impacts. Heavy metal pollution is different from other types of pollution in that it cannot be degraded or decomposed, can persist in the environment for a long time, and has bioaccumulation and biomagnification effects, accumulating in organisms through the food chain [1]. Monitoring and analyzing heavy metals in water quality is an essential means of controlling heavy metal pollution. Water quality monitoring and analysis is one of the important factors determining water quality monitoring work [2] [3]. Through scientific monitoring and analysis of water quality, it is possible to effectively evaluate water quality, warn of risks, support governance, safeguard health, and fulfill international obligations.

In monitoring and analysis, ensuring accurate and reliable data is a key step in uncertainty assessment. Uncertainty assessment can quantify the credibility of test results and help to judge the credibility of data [4] [5]. By evaluating the impact of various factors during the measurement process, such as instrument errors, operational errors, environmental changes, etc., the accuracy of the data can be more comprehensively understood. Can identify the main factors that affect measurement results, optimize monitoring methods and processes, reduce sources of error, and improve measurement accuracy and efficiency. Uncertainty assessment not only provides measurement values, but also gives their possible ranges, helping to explain the results more comprehensively. It is also a good way to measure the management level of inspection and testing institutions [6]. For example, in environmental monitoring, uncertainty assessment can determine whether the concentration of pollutants exceeds the safety limit, enhancing the scientific interpretation of the results. The assessment of uncertainty should be highly valued in monitoring and analysis to ensure accurate and reliable data, providing stronger support for water environment protection.

The purpose of this experiment is to systematically evaluate the uncertainty component of copper element in water quality determined by flame atomic absorption spectrophotometry, analyze the main influencing factors, improve the accuracy of heavy metal monitoring data for water quality monitoring laboratories, promote comparability of results, enhance the interpretation ability of results, improve the competitiveness of laboratories, support technological innovation, and provide reliable uncertainty evaluation methods for water quality monitoring laboratories.

2. Materials and Methods

2.1. Instruments and Reagents

The instruments and equipment used in this experiment are shown in **Table 1**. The operating parameters of the atomic absorption spectrophotometer used for measuring copper content are shown in **Table 2**, and the experimental reagents used are shown in **Table 3**.

Table 1. Equipment status.

Instrument name	Specification and model	Instrument number	Performance status	Remarks
Single label volumetric flask	100 ml, Grade A	—	Verified as qualified	Verification date: March 19, 2023
Single line pipette	1 ml, Grade A	—	Verified as qualified	Verification date: March 19, 2023
Atomic absorption spectrophotometer	PinAAcle 900T	PTDS17041803	Verified as qualified	Verification date: May 13, 2023

Table 2. Operating parameters of instruments.

Element	Cu
Measure wavelength/nm	324.8
Width of passband/nm	0.7
Lamp current/mA	8
Lamp type	HCL

Table 3. Experimental reagent status.

Name	Manufacturer and specifications	Purification treatment method	Remarks
Copper standard solution	Standard Sample Research Institute of the Ministry of Environmental Protection	—	—
Experimental water	Bring your own	—	Ultra pure water
Nitric acid	Tianjin Kemio (MOSS grade) Chemical Reagent Co., Ltd	—	—

2.2. Method Principle

The analytical method for monitoring and analyzing copper elements in water quality is the national environmental protection standard of the People's Republic of China, GB/T7475-1987 [7] "Determination of copper, zinc, lead, and cadmium in water quality by atomic absorption spectrophotometry".

Method principle: Directly inhale the sample or digested sample into the flame to form atoms in the flame. Absorb characteristic electromagnetic radiation, compare the measured absorbance of the sample with the absorbance of the standard solution, and determine the concentration of the measured element in the sample.

2.3. Experimental Steps

Accurately transfer 1ml of standard stock solution into a 100 ml volumetric flask,

dilute to the mark with ultrapure water, and mix well. Choose the appropriate wavelength and adjust the flame, then measure the sample and standard curve.

3. Experimental Steps

3.1. Set the Operating Parameters of the Instrument

Before the sample is drawn into the flame through pre-treatment, the instrument parameters of the atomic absorption spectrophotometer should be set, and the wavelength, passband width, combustion assistance ratio, and flame height should be adjusted to ensure that the inlet pipe is not blocked.

3.2. Preparation of Copper Standard Series Solutions

Measure the absorbance and corresponding concentration of the solution and draw a standard working curve:

1) Standard solution: Transfer 0.50, 1.00, 1.50, 2.00, and 2.50 ml of copper standard solution (100 mg/L) into a 100 ml volumetric flask, add nitric acid solution (1 + 499), dilute to volume, and mix well.

2) Working curve: Measure the absorbance and corresponding concentration of the calibration series solutions in order from low to high concentration. Plot the calibration curve with the absorbance of the solution as the vertical axis and the concentration of copper element solution as the horizontal axis.

3.3. Sample Determination

Take an appropriate amount of water sample and immediately filter it through a 0.45 μm filter membrane to obtain the filtrate for measurement. Find the concentration of copper in the measured solution from the calibration curve.

3.4. Mathematical Model

The formula for calculating the concentration of copper element in water quality samples is:

$$A = k_1 C + k_0$$

In the formula:

A —absorbance;

k_1 —Slope;

C —Concentration (mg/L);

k_0 —Intercept.

4. Uncertainty Component Analysis and Evaluation

4.1. Uncertainty of Standard Solution Used U_{rel1}

Use a 1 mL A-grade pipette to draw copper standard stock solution, place it in a 100 ml volumetric flask (A-grade), and dilute it to the mark with nitric acid solution to prepare copper standard usage solution. This process introduces the uncertainty $u(V_{\text{shift}})$ and $u(V_{\text{volume}})$ of the 1ml pipette and 100ml volumetric

flask:

4.1.1. Uncertainty $u(p)$ Introduced by Standard Reserve Solution

The standard uncertainty $u(p)$ of the copper standard reserve solution, provided as a standard sample with a mass concentration of (100 ± 1) mg/L and a factor of $k=3$, is

$$u(p) = 1(\text{mg/L})/3 = 0.333 \text{ mg/L}$$

The relative standard uncertainty of copper standard reserve solution $U_{rel}(p)$ is:

$$U_{rel}(p) = \frac{u(p)}{p} = 0.33\%$$

4.1.2. Uncertainty Introduced by Standard Liquid Preparation

1) 1 ml pipette introduces standard uncertainty

a) Capacity error u_1 , according to JJG-1996 "Verification Regulations for Commonly Used Glass Containers" [8], the maximum allowable error for 1ml A-grade single standard pipettes is 0.007ml, distributed in a rectangular shape with a factor of $k = \sqrt{3}$, then

$$u_1 = \frac{0.007 \text{ ml}}{\sqrt{3}} = 0.0040 \text{ ml}$$

b) The error introduced by personnel readings u_2 , the uncertainty introduced by personnel readings follows a triangular distribution [9], including the factor $k = \sqrt{6}$, then u_1

$$u_2 = \frac{0.01 \times 1 \text{ ml}}{\sqrt{6}} = 0.00041 \text{ ml}$$

c) The uncertainty introduced by temperature, the temperature during pipette use is different from the calibration temperature, and the maximum temperature variation range of the introduced uncertainty is $\pm 4^\circ\text{C}$. The expansion coefficient of water at 20°C is $2.1 \times 10^{-4}/^\circ\text{C}$ [10], and the inclusion factor is $k = \sqrt{3}$. Therefore

d)

$$u_3 = \frac{1.00 \times 2.1 \times 10^{-4} \times 4 \text{ ml}}{\sqrt{3}} = 0.00048 \text{ ml}$$

$$u(V_{\text{移}}) = \sqrt{u_1^2 + u_2^2 + u_3^2} = 0.0040 \text{ ml}$$

Relative standard uncertainty introduced by 1 ml pipette:

$$U_{rel}(V_{\text{移}}) = \frac{u(V_{\text{移}})}{V_{\text{移}}} = 0.0040$$

2) Uncertainty introduced by 100 ml volumetric flask

The maximum allowable error for a 100 ml A-grade volumetric flask is ± 0.10 ml, as shown in example 4.1.2.

$$u_1 = \frac{0.10 \text{ ml}}{\sqrt{3}} = 0.058 \text{ ml}$$

$$u_2 = \frac{0.05 \times 100 \text{ ml}}{\sqrt{6}} = 0.204 \text{ ml}$$

$$u_3 = \frac{100 \times 2.1 \times 10^{-4} \times 4 \text{ ml}}{\sqrt{3}} = 0.048 \text{ ml}$$

The standard uncertainty introduced by a 100 ml volumetric flask is:

$$u(V_{\text{容}}) = \sqrt{u_1^2 + u_2^2 + u_3^2} = 0.217 \text{ ml}$$

Relative standard uncertainty introduced by 100 ml volumetric flask:

$$U_{\text{rel}}(V_{\text{容}}) = \frac{u(V_{\text{容}})}{V_{\text{容}}} = 0.00217$$

Taking into account the above three factors, the relative uncertainty of the copper standard solution used is:

$$\begin{aligned} U_{\text{rel}1} &= \sqrt{U_{\text{rel}}(p)^2 + U_{\text{rel}}(V_{\text{移}})^2 + U_{\text{rel}}(V_{\text{容}})^2} \\ &= \sqrt{(3.3 \times 10^{-3})^2 + (4.0 \times 10^{-3})^2 + (0.00217)^2} \\ &= 5.62 \times 10^{-3} \end{aligned}$$

4.2. Uncertainty of Standard Curve Fitting $U_{\text{rel}2}$

Using 5 concentrations of copper standard solution, the corresponding absorbance values were measured twice by flame atomic absorption spectrophotometry to determine the linear equation and correlation coefficient. The measurement results are shown in **Table 4**.

Table 4. Absorption values of copper standard series solutions.

Serial number	Concentration C (mg/L)	Absorption A_1	Absorption A_2	Average absorbance A
1	0.5	0.090	0.092	0.091
2	1.0	0.183	0.183	0.183
3	1.5	0.268	0.269	0.268
4	2.0	0.351	0.355	0.353
5	2.5	0.446	0.448	0.447

The regression equation for the working curve of the standard solution calculated from the absorbance values of the copper standard series solution is $A = 0.17761C + 0.00173$, and the correlation coefficient of the working curve is $r = 0.9998$.

Table 5. Determination results of copper content in sample water samples.

Serial number	Sample volume/ml	Fixed volume/ml	Absorbance A	Concentration C /(mg/L)
1	100	100	0.2717	1.52
2	100	100	0.2735	1.53
3	100	100	0.2699	1.51
4	100	100	0.2735	1.53
5	100	100	0.2752	1.54
6	100	100	0.2735	1.53

The average copper content in surface water samples (see **Table 5**) was calculated using the standard curve to \bar{C} be 1.53mg/L. The standard uncertainty introduced by standard curve fitting is:

$$U_C = \frac{S_R}{b} \sqrt{\frac{1}{p} + \frac{1}{n} + \frac{(\bar{C} - \bar{C}_0)^2}{\sum_{i=1}^n (C_{0i} - \bar{C}_0)^2}}$$

In the formula, b is the slope, S_R is the standard deviation of the residual of the regression curve, p is the number of repeated measurements of the sample ($p = 6$), n is the number of points on the regression curve ($n=10$), \bar{C}_0 is the average concentration of the sample to be tested, \bar{C}_{0i} is the average concentration of each point on the regression curve, and is the concentration value of each standard solution. The S_R calculation method is as follows:

$$S_R = \sqrt{\frac{\sum_{i=1}^n [A_{0i} - (a + bC_{0i})]^2}{n - 2}}$$

In the formula, A_{0i} represents the actual absorbance of each standard solution, and $a + bC_{0i}$ represents the theoretical value calculated based on the regression curve.

If the data in the table is substituted to obtain $S_R = 0.0029$ mg/L, then the standard uncertainty introduced by the standard curve fitting is

$$U_c = 0.0099 \text{ mg/L},$$

Relative standard uncertainty

$$U_{rel2} = \frac{U_c}{\bar{C}} = 0.65\%$$

4.3. Uncertainty of Sample Repeatability U_{rel3}

The same sample was continuously measured 6 times under the same conditions, and the average concentration of the samples measured 6 times was 1.53 mg/L, as shown in **Table 6**:

Table 6. Determination results of the same sample under the same conditions.

Measurement frequency	1	2	3	4	5	6
Determination of concentration value (mg/L)	1.52	1.53	1.51	1.53	1.54	1.53

The uncertainty $u(C_i)$ of 6 measurements is:

$$u(C_i) = \frac{\sqrt{\frac{\sum_{i=1}^n (C_i - \bar{C})^2}{n-1}}}{\sqrt{n}} = 0.0045 \text{ mg/L}$$

$$U_{rel3} = \frac{u(C_i)}{\bar{C}} = 0.29\%$$

4.4. Uncertainty of Sampling Volume U_{rel4}

The allowable error of a 20 mL measuring cylinder is $\Delta = \pm 0.5$ mL, including a factor $k = 3$. Therefore, the standard uncertainty of the sampling volume V_2 is:

$$U_{rel4} = U_{V_2} = \frac{0.05}{3} = 0.0167(\text{mL})$$

4.5. Uncertainty Introduced by Instruments U_{rel5}

The atomic absorption spectrophotometer calibration certificate provides copper data with a relative uncertainty of 1% and a factor $k = 2$. Therefore, the relative uncertainty introduced by the analytical instrument is:

$$U_{rel5} = \frac{0.01}{\sqrt{3}} = 5.77 \times 10^{-3}$$

5. Composite Standard Uncertainty

Based on the above data, the main sources of uncertainty in copper determination results for water quality are shown in **Table 7**.

Table 7. Summary of uncertainty in determining copper content in water quality.

Component symbol	Source factor description	Relative uncertainty
$u_{rel}(1)$	Uncertainty introduced by preparing standard solution	5.62×10^{-3}
$u_{rel}(2)$	Uncertainty introduced by standard curve fitting	6.50×10^{-3}
$u_{rel}(3)$	Uncertainty introduced by repeated determination of sample solution	2.90×10^{-3}
$u_{rel}(4)$	Uncertainty introduced by sampling volume	1.67×10^{-2}
$u_{rel}(5)$	Uncertainty introduced by measuring instruments	5.77×10^{-3}

By substituting the results obtained from 3.1, 3.2, 3.3, 3.4, and 3.5 into the formula, the relative standard synthetic uncertainty of copper content in the sample can be obtained

$$U_{rel}(\omega) = \sqrt{U_{rel1}^2 + U_{rel2}^2 + U_{rel3}^2 + U_{rel4}^2 + U_{rel5}^2} = 0.0199$$

The standard synthesis uncertainty is:

$$U_{(Cu)} = \bar{C} * U_{rel}(\omega) = 0.030 \text{ mg/L}$$

6. Expand Uncertainty

According to the guidelines for evaluating measurement uncertainty, in order to make the measurement results comparable to each other, at a 95% confidence level, the extension coefficient $k = 2$ is taken, and the extension uncertainty of copper content in the sample is:

$$U = 2 \times 0.030 = 0.060 \text{ (mg/L)}$$

Therefore, the concentration of copper in the tested sample is (1.53 ± 0.060) mg/L, $k = 2$.

7. Result and Conclusion

The monitoring and analysis of heavy metal elements in water quality is a key step in environmental management and public health protection, and the assessment of uncertainty is the core step to ensure the accuracy and reliability of monitoring data. Ensure the accuracy and reliability of heavy metal monitoring data in water quality, providing strong support for environmental management and public health protection through scientific uncertainty evaluation. In the future, with technological advancements and improved standards, uncertainty assessment will play a more important role in water quality monitoring.

This article uses flame atomic absorption spectrophotometry to determine the copper content in water samples. During the analysis process, five uncertainty components were considered, including solution, standard curve, sample repeatability, sampling volume, and experimental instruments, and a mathematical model was established for analysis. Study its impact on measurement results. The experimental results indicate that the copper content in the water quality sample is (1.53 ± 0.060) mg/L, and the sampling volume and standard curve measurement are the main sources of uncertainty. Optimizing the use of measuring instruments in experiments and improving the operational skills of operators can effectively reduce uncertainty and improve measurement accuracy.

In the future actual sample measurement process, in order to ensure the accuracy and reliability of experimental results, attention should be paid to the following aspects to minimize various uncertainty components:

1) Standard solution preparation: Use certified standard substances and control the experimental temperature. Choose high-precision glass containers. Standardize the operation of testing personnel and improve the configuration accuracy of

each concentration point on the standard curve.

2) Standard curve fitting: After analysis, the smaller the uncertainty introduced by curve fitting, the closer the concentration of the measured element is to the average value of the standard solution. When conducting sample analysis, the actual sample can be initially measured, and then a standard solution can be selected to determine the appropriate concentration of the sample. Simultaneously increase the measurement frequency of standard solutions and actual samples to reduce the uncertainty caused by curve fitting.

3) Instrument maintenance: To ensure the stability and sensitivity of the instrument, regular maintenance, periodic inspections, calibration, and calibration of the instrument equipment are carried out according to regulations.

The accuracy and reliability of uncertainty and measurement results can be improved through the above measures.

Conflicts of Interest

The authors declare no conflicts of interest.

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