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РОЗРОБКА ШВИДКОГО, ПРОСТОГО ТА НЕДОРОГОГО ТЕСТУ ДЛЯ ВИЗНАЧЕННЯ ВМІСТУ ЗАЛІЗА В ПОВЕРХНЕВИХ І МОРСЬКИХ ВОДАХ

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DEVELOPMENT OF A QUICK, SIMPLE AND LOW-COST TEST FOR IRON CONTENT DETERMINATION IN SURFACE AND MARINE WATER

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Військові дії на території України загострили проблему моніторингу водних об'єктів та зумовили необхідність у створенні швидкого, простого й недорогого методу скринінгу феруму за дефіциту лабораторного контролю. Об'єктом дослідження є індикаторна (колориметрична) тест-система для експрес-визначення вмісту заліза у поверхневих і морських водах у польових умовах. Для вибору складу тесту на модельних водах із вмістом $Fe(III)$ 1 та 5 mg/dm^3 порівняли дію двох хромогенних реагентів ($KSCN$ і сульфосаліцилова кислота) та регуляторів pH (10% NH_4OH і 5N H_2SO_4) за спектрофотометричними характеристиками. Встановлено, що для обох концентрацій феруму найінтенсивніше та найбільш контрастне забарвлення забезпечує комбінація $KSCN + H_2SO_4$. Система із сульфосаліциловою кислотою формує менш контрастний сигнал, а відтінки жовтого кольору у лужному середовищі є складними для надійного візуального розпізнавання та детектування. Показано, що забарвлення тіоціанатного комплексу є достатньо стабільним для польового зчитування: протягом перших 10 хв після змішування оптична густина зменшується менш ніж на 5% і візуально не фіксується. Розроблено колірну шкалу в діапазоні 0–10 mg/dm^3 $Fe(III)$ і протокол тестування, який полягав в додаванні 25 cm^3 проби, 2,5 cm^3 5N H_2SO_4 та 1 г $KSCN$ із зчитуванням через ~2 хв і порівнянням зі шкалою. Отримані в результаті досліджень тест-системи рекомендовано для оперативного моніторингу заліза у річках, прибережних та морських водах, контролю водозаборів і очисних споруд, виїзних обстежень після аварійних/воєнних впливів та громадського моніторингу. Тест-набір може бути реалізовано у форматі «циліндр – ампула – саше – шкала», що мінімізує дозування реагентів і забезпечує придатність для роботи поза лабораторією. Результати можуть бути задокументовані фотографуванням смартфоном і подальшим RGB-кодуванням.

Ключові слова: визначення заліза, $Fe(II)/Fe(III)$, тіоціанат, колориметричний тест, польовий моніторинг, експрес-аналіз, смартфон-колориметрія.

Military operations in Ukraine have intensified the challenge of monitoring water bodies and have created a strong demand for a rapid, simple, and low-cost method for iron screening under limited laboratory control. The object of research is an indicator colorimetric test system intended for fast determination of iron concentration in surface and marine waters under field conditions. To select the test formulation, two chromogenic reagents, potassium thiocyanate (KSCN) and sulfosalicylic acid, as well as pH adjusters, 10% NH₄OH and 5N H₂SO₄, were compared using spectrophotometric characteristics in model waters containing 1 and 5 mg/L of Fe(III). It was established that, at both iron levels, the KSCN and H₂SO₄ combination provides the highest colour intensity and the best visual contrast. The sulfosalicylic acid system produces a less contrasted signal, and the yellow shades formed in alkaline medium are difficult to distinguish reliably by visual inspection and therefore complicate detection. The thiocyanate complex was shown to be sufficiently stable for field readout since during the first 10 minutes after mixing the absorbance decreases by less than 5% and the change is not visually perceptible. A colour scale covering 0 to 10 mg/L of Fe(III) was developed together with a test protocol that involves adding 25 ml of the sample, 2.5 ml of 5N H₂SO₄, and 1 g of KSCN, followed by reading after approximately 2 minutes by comparing the solution colour with the scale. The developed test systems are recommended for rapid monitoring of iron in natural waters. The kit can be implemented in a “cylinder – ampoule – sachet – scale configuration”, which reduces reagent dosing steps and supports use outside the laboratory. Results can be documented using smartphone photography followed by RGB based colour coding.

Keywords: iron detection, Fe(II)/Fe(III), thiocyanate, colorimetric test, field monitoring, rapid analysis, smartphone colorimetry.

1. Introduction

As a result of the Russia-Ukraine war, the condition of many natural water bodies in Ukraine has deteriorated significantly. Flooding of military vehicles, ammunition, missiles, mines, and damaged bridge structures adversely affects water quality [1, 2]. Ammunition may contain up to 95–97% lead, about 2% tin, and smaller amounts of nickel, zinc, copper, and manganese [3]. Some ammunition types also contain mercury in detonator capsules [4]. Corrosion of metal structural components leads to water contamination with iron compounds and various heavy metals. In addition, frequent power outages in the Donbas region have increased the risk of contamination of water sources by mine waters due to failures of pumping equipment [5]. In marine [6] and coastal [7] waters, deterioration in water quality is also frequently observed due to riverine inputs, shoreline erosion, resuspension of bottom sediments, port activities, damage to coastal infrastructure, and military operations at sea [8]. Clear examples of war related metal pollution include the concentrations of these components in the Molochna River water (Zaporizhzhia region, Ukraine) and in the bottom sediments of a lake in Bucha district (Kyiv region, Ukraine) [1, 9, 10]. In the Molochna River, copper, lead, chromium, and nickel contents markedly exceed the maximum permissible concentrations by factors of 950, 20.7, 4.8, and 10.6, respectively [9]. In bottom sediments from Bucha district, the contents of iron, copper, manganese, and aluminium

increased sharply after the onset of active hostilities in the region by factors of 4.8, 2.2, 4.8, and 2.9, respectively [10].

Most Ukrainian drinking water treatment plants rely on surface waters for tap water production [11, 12]. However, the war has severely disrupted water quality monitoring systems, and in some regions, monitoring is not performed at all, which increases the risk of producing insufficiently treated water [13]. In particular, drinking water contaminated with heavy metals can cause numerous adverse health effects that are often irreversible [14, 15].

Therefore, especially under wartime conditions, operational water quality control in Ukraine is increasingly shifting from a purely laboratory-based approach to a hybrid model. In this model, the laboratory retains the role of reference verification, whereas primary screening and a part of routine measurements are carried out directly at sampling sites or supported by remote sensing. This is particularly relevant for large basins, coastal zones, and areas with limited access to laboratory infrastructure [16, 17]. These circumstances make the development of rapid, simple, and low-cost tests for pollutant determination highly important. Commercial test systems are currently available on the market, yet their composition and operating principles are often undisclosed, and their cost remains high. This justifies the need for an alternative low-cost method that can be produced locally in Ukraine and motivates the development of new tests that enable iron determination in water to be simple in use, affordable, and widely accessible. The importance of an iron detection test system is associated with the fact that iron can serve as a direct marker of corrosion driven deterioration of pipes and reservoirs and of changes in redox conditions. A pronounced increase in iron concentration that is atypical for a given water body may also be an indirect indication of elevated levels of other metal ions because iron and heavy metals can enter the water simultaneously during corrosion of metal alloys [18]. Iron can additionally act as a supporting indicator of bottom sediment mobilisation, particularly in areas affected by hydrodynamic disturbances [19, 20]. It can also serve as an operational parameter to assess treatment performance during coagulation, aeration, filtration, and related processes [21, 22].

Consequently, the goal of a rapid iron test for surface and marine waters is not to replace high precision methods such as ICP MS or AAS, but to provide a fast on site decision while maintaining sufficient accuracy within threshold concentration ranges.

A wide variety of chromogenic components has been reported for detecting iron compounds in water, including 1-(5-bromo-2-pyridylazo)-2-naphthol-6-sulfonic acid, the disodium salt of 1-nitroso-2-naphthol-3,6-disulfonic acid, sulfosalicylic acid, o-phenanthroline, ammonium or potassium thiocyanate, 2-naphthylcarboxymethylene citrate, ferene S, and others [23, 24]. 1-(5-bromo-2-pyridylazo)-2-naphthol-6-sulfonic acid, the disodium salt of 1-nitroso-2-naphthol-3,6-disulfonic acid, and many other highly sensitive chromogenic compounds are very expensive. This makes indicator systems based on these reagents economically unattractive because high costs reduce market demand.

Ferrozine is widely used for Fe(II) determination due to the high molar absorptivity of its complex and good selectivity. For total iron in mixtures of Fe(III) and Fe(II), Fe(III) is reduced to Fe(II) prior to measurement. Practical procedures for

natural waters, including marine waters, often rely on ferrozine and describe how to distinguish Fe(II) and Fe(III) by measurements before and after the reduction step [25]. In saline seawater, part of the iron can be masked within organic complexes [26], including natural organic matter and some anthropogenic organic pollutants [27], which may hinder direct colour development [28]. Ready to use commercial kits from Hach based on ferrozine are applied in the $\text{mg} \cdot \text{L}^{-1}$ range, for example with a working range of 0.009–1.400 $\text{mg} \cdot \text{L}^{-1}$ [29].

Another reagent frequently used for iron determination is 1,10-phenanthroline. This compound contains a ferrioxalate forming group and can produce a stable complex with ferrous iron, Fe^{2+} , providing stable absorption at 510 nm [30]. For total iron determination, Fe(III) is reduced to Fe(II) prior to complexation [31, 32]. Traditionally, phenanthroline based metal ion detection is performed by absorption spectroscopy and the method is often used in routine monitoring [33]. In particular, study [34] examined a sensitive and non-destructive approach for qualitative and quantitative iron analysis using the phenanthroline– Fe^{2+} complex within a working range of 0.05 to 10 $\mu\text{g} \cdot \text{mL}^{-1}$ of iron(II). In that study, the colour intensity of the phenanthroline– Fe^{2+} complex increased with increasing Fe^{3+} concentration, as determined from changes in Raman spectra and a rapid colour shift from colourless to orange red. Several studies have also demonstrated iron detection using paper based analytical devices. For example, study [35] fabricated a microfluidic paper based analytical device using photolithography to create hydrophilic and hydrophobic zones and enabled iron detection using 1,10-phenanthroline. The method achieved a limit of detection (LOD) of 3.96 μM and a limit of quantification (LOQ) of 13.8 μM . However, this approach has several limitations. These include the complexity of device fabrication, the need for high initial setup costs, challenges in scaling production for commercial use, and the potential environmental impact of some chemicals involved in manufacturing [36].

When detecting iron in water, an important factor is that Fe(III) is the predominant form in surface waters [37] due to the presence of dissolved oxygen [38]. Dissolved oxygen reacts with Fe(II), converting it to Fe(III) [39]. Therefore, a test should change colour either in response to both iron forms or selectively to Fe(III). For this study, thiocyanate and sulfosalicylic acid were selected as reagents for iron determination. Thiocyanate ions form a coloured compound with Fe(III), and potassium persulfate can be used when oxidation of Fe(II) to Fe(III) is required [40]. Depending on the solution pH, sulfosalicylic acid can be applied either for iron determination under conditions that favour one form or for total determination of both forms [41]. In acidic medium, Fe(III) reacts with thiocyanate to form a red orange complex in the visible region of 450–530 nm with a maximum near 450 nm [42]. The use of these reagents for iron determination is cost effective, results in rapid colour development, and enables a user friendly test system that can incorporate smartphone based readout, given the widespread availability of smartphones. For example, study [42] used a smartphone as a photometer for Fe(III)–SCN determination and reported linearity in the range 10–80 $\text{mg} \cdot \text{L}^{-1}$, with LOD of 0.1 $\text{mg} \cdot \text{L}^{-1}$ and LOQ of 0.3 $\text{mg} \cdot \text{L}^{-1}$, demonstrating the feasibility of the approach. Microfluidic paper based analytical device for Fe(III) detection using thiocyanate to form a red brown $\text{Fe}(\text{SCN})^{2+}$ complex is a novel approach in water quality monitoring [43]. Colour change in this method was analysed from

smartphone images [43]. The method showed a linear response between 10 and 100 mg · L⁻¹ Fe(III), although key performance parameters such as LOD and LOQ were not reported.

Despite the existing literature, most reported approaches target relatively high Fe(III) concentrations and do not consistently account for the characteristics of natural waters, including seawater salinity and background colour. This limits their suitability for rapid screening within concentration ranges typical for water bodies, where a simple procedure, a temporally stable signal, and a clear readout without complex equipment are required. For these reasons, it is reasonable to develop a unified low-cost test system optimised for field conditions and applicable to both surface and marine waters.

The object of research is an indicator colorimetric test system intended for fast determination of iron concentration in surface and marine waters under field conditions.

The aim of this research is to develop a simple and inexpensive test for rapid determination of total iron in surface and marine waters.

To achieve this aim, it was necessary:

- 1) to select an optimal combination of indicator reagents that provide an intense colour response with Fe(III) ions and, when required, with Fe(II) after conversion;
- 2) to evaluate the temporal stability of the selected system within a period sufficient for field readout;
- 3) to create a colour scale for estimating iron concentration under field conditions.

2. Materials and Methods

To optimise the formulation of the test kit, two model water samples were prepared by adding iron(III) chloride to obtain iron concentrations of 1 mg · L⁻¹ and 5 mg · L⁻¹ (as Fe). A 100 g · L⁻¹ potassium thiocyanate (KSCN) solution and a 10% sulfosalicylic acid solution were evaluated as chromogenic components. A 10% ammonia solution (NH₄OH) was used to create alkaline conditions, and a 5N sulfuric acid solution (H₂SO₄) was used to create acidic conditions. Table 1 summarises the reagent combinations investigated at 1 mg · L⁻¹ and 5 mg · L⁻¹ iron to select the optimal test formulation. Each mixture was prepared in a 50 mL volumetric flask by adding the reagents according to Table 1 and diluting to volume.

For each prepared mixture, an absorbance spectrum was recorded using a UV-2600i UV-VIS spectrophotometer (Shimadzu) in the visible range (380–780 nm) with a 1 cm optical path length cuvette. This approach enabled a quantitative assessment of colour intensity and a direct comparison of the performance of the tested reagents.

Table 1

Combinations of reagents for model solutions with different iron contents

No.	Fe content, $\text{mg} \cdot \text{L}^{-1}$	KSCN, mL	Sulfosalicylic acid, mL	Ammonia, mL	Sulfuric acid, mL
1	1	5	–	–	–
2	1	10	–	–	–
3	1	5	–	–	5
4	1	–	5	–	–
5	1	–	5	5	–
6	1	–	5	–	5
7	5	5	–	–	–
8	5	10	–	–	–
9	5	10	–	–	5
10	5	–	5	–	–
11	5	–	5	5	–
12	5	–	5	–	5

After selecting the optimal test composition, a colour scale for visual iron determination was produced. A series of Fe(III) model solutions was prepared with concentrations of 0, 0.05, 0.1, 0.2, 0.3, 0.5, 0.8, 1.0, 2.0, 5.0, and 10.0 $\text{mg} \cdot \text{L}^{-1}$. Each sample (25 mL) was transferred into a transparent vessel, followed by the addition of 2.5 mL of 5N H_2SO_4 and 1 g of KSCN as a dry portion. The vessel was closed and vigorously shaken until the salt fully dissolved. The vessel was then placed on a white background and photographed from above using a digital camera. The images were white balanced, and the colour codes (RGB) were determined using a graphics editor (the free online editor Photopea). In this way, a set of reference colour shades was established for different iron concentrations.

3. Results and Discussion

3.1. Selection of an optimal combination of indicator reagents for Fe(III) and Fe(II)

Fe(III) ions form thiocyanate complexes of variable composition in solution, ranging from $[\text{Fe}(\text{SCN})]^{2+}$ to $[\text{Fe}(\text{SCN})_3]$. At high iron and thiocyanate concentrations, the solution develops an intense red colour, whereas at lower concentrations it appears orange-brown. Increasing the KSCN content in the system enhances colour intensity because a larger amount of the $[\text{Fe}(\text{SCN})]^{2+}$ complex is formed (Fig. 1). Acid addition, which shifts pH toward acidic values, also promotes Fe(III) thiocyanate complex formation since it suppresses iron hydrolysis and prevents precipitation of $\text{Fe}(\text{OH})_3$.

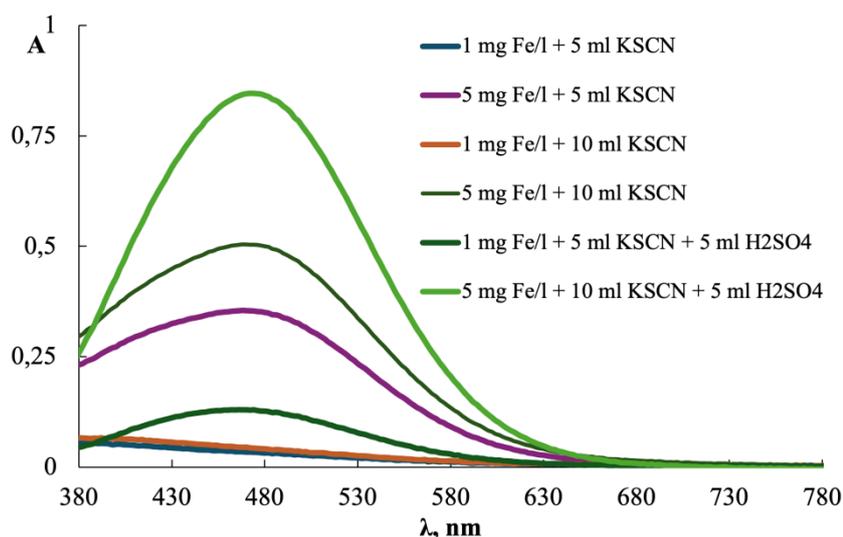


Fig. 1. Effect of KSCN and sulfuric acid content on colour intensity

The absorbance spectra in Fig. 1 show that the most intense colour among all thiocyanate-based mixtures is obtained with the KSCN and H₂SO₄ combination, both at 1 mg · L⁻¹ Fe and at 5 mg · L⁻¹ Fe. Therefore, combining thiocyanate with a strong acid is an appropriate strategy to achieve a bright and stable colour response.

Sulfosalicylic acid can form complexes with both Fe(III) and Fe(II). The complex colour depends on pH. In acidic solution, a violet-red complex is formed mainly with Fe(III), whereas at alkaline pH a yellow complex is produced that corresponds to the total content of all iron forms [44]. In practice, excess ammonia (10% NH₄OH) was added to obtain the yellow colour, and several drops of 5N H₂SO₄ were used to obtain the violet colour. Spectral measurements (Fig. 2) indicated that, at the same iron concentration, the yellow complex formed under alkaline conditions exhibits a substantially higher absorbance than the violet complex formed in acidic medium. This suggests that small iron concentrations are more effectively detected in alkaline solution when total iron is targeted because the colour intensity is higher. However, yellow shades of different saturation are difficult to discriminate visually, which makes this option less convenient for practical colorimetric testing.

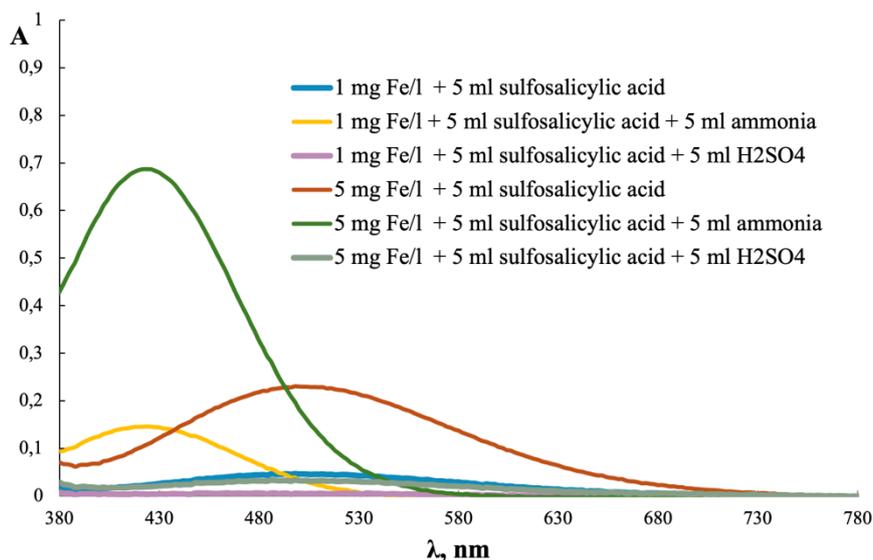


Fig. 2. Effect of sulfosalicylic acid content and pH regulators on colour intensity

For comparison, Fig. 3 presents the spectra of the most effective reagent combinations from each group, namely the thiocyanate system with sulfuric acid and the sulfosalicylic system with ammonium hydroxide.

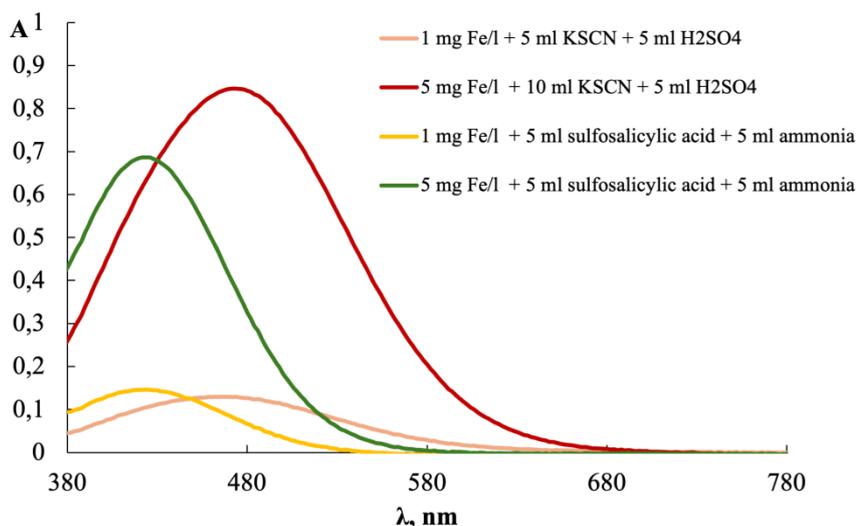


Fig. 3. Effect of the type of chromogenic component on the detection of iron

Fig. 3 indicates that both the absorbance maximum and the overall colour intensity are markedly higher for the Fe(III) thiocyanate complex. Although sulfosalicylic acid can, in principle, enable simultaneous determination of both iron forms under alkaline conditions, it provides lower sensitivity. The peak absorbance values are smaller, and the human eye distinguishes yellow tones less reliably than the sharp red orange tones produced by the thiocyanate complex. For these reasons, the thiocyanate system

operated in acidic medium was selected for the developed test as the most sensitive and visually clear option.

The proposed method enables rapid estimation of total dissolved iron, mainly present as Fe(III), directly under field conditions. If the tested water may contain a significant fraction of Fe(II), for example in some groundwaters, the protocol can be modified by adding an oxidant before thiocyanate addition. Potassium persulfate, $K_2S_2O_8$, can be used and the sample should be allowed to stand for several minutes to convert Fe(II) to Fe(III). This ensures that all dissolved iron is determined as the Fe(III) thiocyanate complex.

3.2. Evaluation of the temporal stability of the selected system for field readout

An additional practical parameter for the test system is the stability of the developed colour because the user must have sufficient time to compare the sample shade with the reference scale. For the selected KSCN and 5N H_2SO_4 formulation, the change in colour intensity with time was evaluated (Fig. 4).

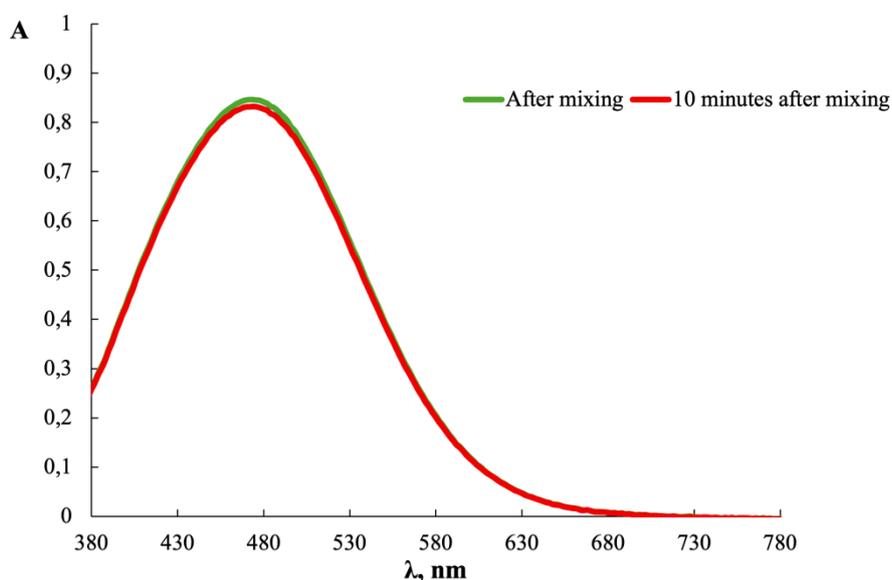


Fig. 4. Effect of time on colour intensity for an indicator system based on potassium thiocyanate and sulfuric acid

The results show that during the first 10 minutes after reagent mixing, only a minor decrease in absorbance is observed, below 5%, and this change does not affect visual colour perception. Subsequently, up to 30 minutes, the colour remains essentially unchanged. Therefore, the user has sufficient time, at least 10 minutes, to perform visual analysis of the sample.

3.3. Creation of a colour scale for iron concentration estimation under field conditions

At the final stage, the kit configuration was simplified to minimise the number of handling steps. Instead of using a thiocyanate solution, thiocyanate was added in solid form as pre dosed salt portions. The final test kit includes a transparent graduated

cylinder with a cap; plastic ampoules each containing 2.5 mL of 5N H₂SO₄, sealed sachets containing 1 g portions of KSCN, and a printed colour scale for different iron concentrations (Fig. 5). To improve the reproducibility of visual interpretation and enable digital documentation, the colour scale was unified using RGB colour coding (Table 2). This standardisation step reduces subjectivity during field readout and supports consistent comparison across different operators and measurement campaigns.

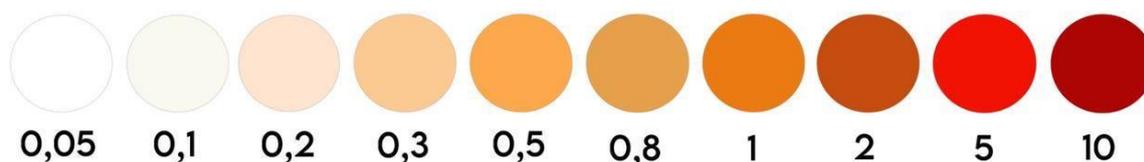


Fig. 5. Colour scale for waters with different iron content ($\text{mg}\cdot\text{L}^{-1}$)

Table 2

Correlation between Fe(III) concentrations and RGB reference codes

Iron content ($\text{mg}\cdot\text{L}^{-1}$)	0.05	0.1	0.2	0.3	0.5	0.8	1	2	5	10
RGB codes	255, 253, 252	249, 249, 239	255, 228, 207	251, 202, 146	253, 168, 77	231, 159, 75	235, 122, 18	199, 76, 16	241, 18, 3	173, 5, 4

The operating procedure is as follows. A 25 mL aliquot of the water sample is poured into the cylinder, the contents of one acid ampoule and one thiocyanate sachet are added, the cylinder is capped, and the mixture is shaken until the salt dissolves. After approximately 2 minutes, the cylinder is placed on a white background next to the scale and the solution colour is visually compared with the nearest reference circles. The iron concentration is estimated from the closest matching shade.

The proposed method enables rapid estimation of total dissolved iron, mainly present as Fe(III), directly under field conditions. If the tested water may contain a significant fraction of Fe(II), for example in some groundwaters, the protocol can be modified by adding an oxidant before thiocyanate addition. Potassium persulfate, K₂S₂O₈, can be used and the sample should be allowed to stand for several minutes to convert Fe(II) to Fe(III). This ensures that all dissolved iron is determined as the Fe(III) thiocyanate complex.

The obtained results indicate that the developed thiocyanate-based test system provides an intense, high contrast, and sufficiently time stable analytical signal while requiring a minimal number of handling steps and a low consumption of reagents, which is a key advantage for field applications. At the same time, 5 N H₂SO₄ is used as a pH regulator in the proposed procedure. The method also relies on pre-dosed reagents. Therefore, the procedure requires not only analytical validation but also an environmental assessment. This is important because water quality methods are increasingly expected to follow green analytical chemistry principles. In this context, it

is appropriate to quantify the greenness of the proposed approach in terms of safety, resource efficiency, waste generation, and simplification of operations.

For an integral assessment of the method impact on the environment and human health, the study employed the Analytical GREENess (AGREE) tool [45]. This calculator implements an approach based on the 12 principles of green analytical chemistry and enables a standardised evaluation of a method across a set of criteria related to reagent use, toxicity, energy consumption, number of procedural steps, potential for miniaturisation, and prospects for automation. Each principle is assigned a score on a unified 0 to 1 scale, after which a weighted overall score is calculated, and the result is visualised as a pictogram that reports both the total score and the contribution of each individual criterion (Fig. 6).

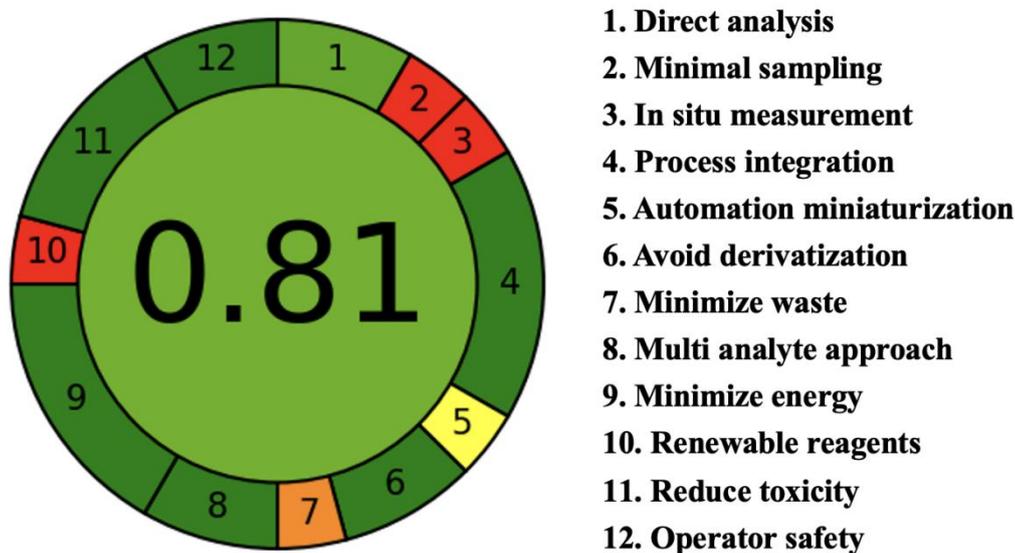


Fig. 6. Diagram of evaluation the environmental and occupational hazards associated with a using thiocyanate based colorimetric method based on the 12 principles of Green Analytical Chemistry

For the proposed thiocyanate based colorimetric method, an overall AGREE score of 0.81 was obtained, indicating a generally high level of compliance with the principles of green analytical chemistry (Fig. 6). The pictogram analysis shows that the lowest values correspond to principles 2, 3, and 10, meaning that the method still requires a certain number of samples, does not fully enable in situ measurements, and relies on reagents that are not derived from renewable sources. Medium scores were obtained for principles 5 and 7, which indicates potential for further miniaturisation and automation, as well as for reducing the generation of analytical waste and improving its management. At the same time, high scores for the remaining principles demonstrate that the method has low energy demand, avoids derivatisation steps, involves a minimal number of operations, and provides an adequate level of operator safety when the acidic reagent is handled properly.

Therefore, the developed test system can be considered an environmentally acceptable green solution for rapid field monitoring of iron in surface and marine waters. Further improvements should reduce the number of samples required. They should also expand the possibility of in situ measurements. In addition, some reagents could be replaced with more renewable or less resource intensive alternatives.

The developed thiocyanate-based kit provides a rapid, low cost, and operationally simple tool for on-site screening of iron in surface and coastal or marine waters. In practice, it can be used for emergency surveys after war related or accident-related impacts, for routine checks at water intakes and treatment facilities, and for quick identification of areas that require confirmatory laboratory analysis. The pre dosed cylinder, ampoule, and sachet format reduces dosing errors and supports use by non-specialist personnel, while RGB standardisation enables documentation and comparison of results between operators and monitoring campaigns.

The proposed approach is primarily intended for screening and semi-quantitative assessment of the presence of iron ions in water, so its accuracy depends on correct visual comparison, lighting conditions, and the operator. The composition of the water being tested can affect color development due to turbidity, background color, and iron complexation with dissolved organic matter, especially in saline waters. In waters where there is a significant amount of Fe(II), an additional oxidation step may be necessary to convert Fe(II) to Fe(III) before adding thiocyanate. In addition, safe handling and transportation of 5 N H₂SO₄ must be ensured, and additional validation must be performed to quantitatively assess method performance indicators such as accuracy, deviation from the reference method, and sensitivity to common interfering ions.

Further work should include the development of a standardized workflow for smartphones. For example, automated RGB processing can reduce subjectivity and improve applicability in the field. Further optimization should focus on more environmentally friendly and safer operation by reducing acidity, minimizing waste, and seeking alternative reagents or formats that improve AGREE principles related to sampling, on-site measurement, and renewable materials.

4. Conclusions

1. In model Fe(III) solutions at 1 and 5 mg · L⁻¹, potassium thiocyanate and sulfosalicylic acid were compared spectrophotometrically in the presence of 10% NH₄OH and 5N H₂SO₄. It was established that the KSCN and H₂SO₄ combination provides the highest signal intensity and the best visual contrast at both iron levels, which is essential for reliable field readout. This result justifies the selection of the thiocyanate route as the primary sensing chemistry for the developed kit.

It was found that adding H₂SO₄ to the thiocyanate system enhances the analytical response and reduces the risk of Fe(III) hydrolysis, thereby ensuring stable formation of a red orange complex. Sulfosalicylic acid in alkaline medium produces a more intense yellow signal, yet yellow shades are more difficult for the operator to discriminate, making the thiocyanate system more practical for visual detection. Accordingly, the proposed approach prioritises colour discriminability and operational robustness rather than maximum absorbance alone.

2. For the KSCN and 5N H₂SO₄ system, the absorbance decreased by less than 5% during the first 10 minutes and did not affect visual perception, which provides a sufficient time window for reading and comparing the sample colour with the reference scale. The colour stability up to 30 minutes further supports use under field conditions where immediate readout may not always be possible.

3. A semi quantitative colour scale for Fe(III) determination in the range 0 to 10 mg·L⁻¹ was established. White balance correction and RGB based colour coding were proposed to standardise reference colours and improve comparison reproducibility. This digital documentation step reduces subjectivity and enables retrospective verification of results and data sharing between operators.

A test kit format based on a cylinder, ampoule, sachet, and printed scale was developed together with an operating protocol that includes adding 25 mL of sample, 2.5 mL of 5N H₂SO₄, and 1 g of KSCN, followed by colour reading after approximately 2 minutes. The method is suitable for rapid monitoring of iron in surface waters and coastal or marine waters and for operational control of water intakes and treatment facilities. The kit design minimises dosing errors by using pre measured portions and reduces the number of handling steps, which increases usability for non-specialist personnel. For waters with elevated Fe(II), preliminary oxidation with potassium persulfate to Fe(III) is recommended. This optional step expands the method applicability to reducing matrices such as certain groundwaters and ensures that total dissolved iron is quantified via the Fe(III) thiocyanate complex.

Conflict of interest

The authors declare that they have no conflicts of interest in relation to this research, including financial, personal, authorship, or other, that could affect the paper and its results presented in this article.

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Data availability

Data will be made available on reasonable request.

Authors' contributions

Marta Litynska: Conceptualisation, Methodology, Investigation, Formal analysis, Writing – original draft; *Mariia Dubenets*: Investigation, Visualisation; *Svitlana Kyrii*: Writing – reviewing and editing, Visualisation, Project administration, Funding acquisition.

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