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Monitoring water quality: a challenge for spectroscopic technology

Water is vital for human survival and its quality is critical for human health, environmental conservation, and food security. However due to the rapid population growth in the last century, the excessive use of agricultural fertilizers to meet our increasing food demands, and the discharge of various industrial pollutants into rivers and oceans, we have been compromising the quality of our water supply [2].

For these reasons, monitoring water quality has become essential in two main areas:

- Environmental monitoring
- Drinking water quality monitoring

Environmental monitoring

When a body of water becomes too rich in nutrients such as nitrogen and phosphorus due to the impact of human activities, the consequent reduction in oxygen levels causes the death of aquatic life. This poses a challenge to conservation efforts and our food supply [1,2].

Monitoring wastewater quality serves two purposes: early detection of pollution events and continuously ensuring compliance with regulations at treatment facilities [7]. For example, hospitals and pharmaceutical plants generate large amounts of concentrated antibiotic wastewater that needs to be treated and analyzed before being released into the environment [1,14].

Drinking water monitoring

Water utilities are committed to meeting the drinking-water standards which are often derived from the World Health Organization drinking water quality guidelines. Water quality monitoring and treatment are two vital aspects of water quality management systems to detect hazards and events that can compromise its quality and provide operational control for assuring safe and reliable drinking water as preventive measures [3].

Conventional methods for water analysis

When it comes to monitoring water quality, a routine sampling program is typically utilized, which involves collecting and transporting water samples to a laboratory for analysis. However, this approach only partially explains water quality over time and may not accurately capture short-term fluctuations. Moreover, feedback from the laboratory is often delayed, making it difficult to respond quickly to any water incidents that may occur [4].

Currently, methods for assessing water quality parameters consist primarily of chemical, biological, and physical approaches [5]. The main chemical methods include titration analysis and electrochemical analysis, which are used to determine pollutant concentrations in a laboratory setting. However, these methods require bulky and expensive equipment, and a large number of reagents which can result in secondary pollution.
Biological methods involve enrichment analysis and biosensor technology but suffer from lower accuracy and sensitivity compared to other methods. The results from the chemical and biological methods are also generally not provided in real-time [6].

UV-Vis spectroscopy for online water monitoring

On the other hand, physical methods consist of spectral remote sensing technology in the UV and visible wavelengths. In fact, the principle of UV-Vis spectrophotometry relies on the correlation between the absorption of specific light wavelengths by a substance and its concentration [8].

Thanks to software particle compensation, spectrophotometry generally does not require sample filtrations, it is reagent free and allows fast measurements of water quality in real-time. This method has been increasingly utilized in the realm of rapid water quality assessment in recent years [6].

Among the parameters that can be measured using UV-Vis spectrophotometers, we can commonly find color, nitrate, Depleted Oxygen Content (DOC), Total Oxygen Content (TOC) and the spectral absorption coefficient SAC254 (sometimes referred as UV254). In recent years, additional parameters have been included in water quality monitoring using online UV-Vis spectrophotometers [8], such as measurements of dissolved organic matter [9], chemical oxygen demand (COD) in water bodies [10], and disinfectant in drinking water [11].

Single-wavelength and multiwavelength detectors

There are mainly two types of spectral sensors used in water analysis: single wavelength (SW) sensors and spectrophotometers.

SW sensors generally consist of a bandpass-filtered single photodetector (Silicon Photodiode or Avalanche Photodiode) and a light source that emits in the targeted wavelength and is absorbed by the substance to be detected. However, spectrophotometers use a broadband light source, a diffractive grating that separates light into its wavelengths components and directs it towards a linear array photodetector.

Online SW UV-Vis instruments can determine concentrations of a specific water parameter (most typically UV254, nitrate, or nitrite) based on the absorbance of a selected single wavelength [12]. In comparison, UV-Vis spectrophotometers measure the absorbances of a certain wavelength band. These sensors produce spectral fingerprints which are used to determine concentrations of water quality parameters based on the instrument's built-in algorithms [13].

Generally, when comparing the performance of full-spectrum and SW sensors, the latter can measure parameter variations during certain periods but may not compensate for the particle effect accurately, specifically when comparing the results with the standard laboratory procedures and measurements. On the contrary, spectrophotometers provide better particle compensation and can be calibrated to specific locations with higher accuracy. They are better for precise applications, such as real-time water and treatment process monitoring [13].

Light sources for UV-Vis spectroscopy

When using a UV-Vis spectral or full-spectrum sensor, it is crucial to choose the most suitable broadband light source. The main requirements for a light source to be used in UV-Vis spectrophotometry are:

- **Suitable spectrum:** the light source needs to emit in the absorption wavelengths of the target molecules to be detected.
- **Brightness:** a high-radiant intensity at the target wavelengths will maximize the sensitivity of the measurement for a specific parameter.
- **Reliability:** flash-to-flash stability, even under environmental changes, guarantees the highest repeatability and accuracy for the measurement.
- **Warm-up time:** short to no warm-up times will make the measurement readily available and accurate at any moment.
- **Lifetime:** longer emitter lifespans reduce maintenance costs, especially when the online sensor is remotely located.
- **Power consumption:** low power consumption will allow for integration of the light source into a battery-powered device that can be handheld or deployed in remote areas.
- **Compactness:** a limited lamp footprint enables the integration into a portable device or narrow spaces.

Although LEDs have been adopted in all sorts of applications in the last decades due to their fast repetition rate, compactness, long lifetimes, and low cost, these light emitters are not as valuable in UV-Vis spectrophotometry applications. In fact, they emit narrow-spectrum light and they generally come in a limited number of available wavelengths.

The most used light sources in spectrophotometry for water analysis are instead broadband emitters like Deuterium Lamps and Xenon Flash Lamps.

While Deuterium lamps generally show a lower peak-to-peak variation, their emission spectrum is limited between 180 nm and 370 nm, they require long warmups and show shorter lifetimes. For these reasons, Deuterium Lamps are generally preferred for integration in lab-based benchtop devices.

Nonetheless, Xenon Flash Lamps offer a wider wavelength range that extends from the UV to the IR allowing for a higher number of water parameters to be detected simultaneously.

Hamamatsu's Xenon Flash lamps for portable spectrophotometers

Using their unique know-how in vacuum device fabrication and electronics integration, Hamamatsu Photonics has developed the most advanced Xenon Flash Lamps for UV-Vis-NIR portable spectrophotometry and online water monitoring.

Xenon flash lamps

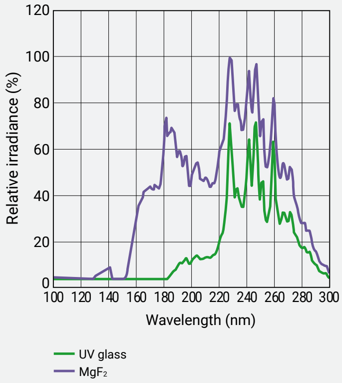
Trigger sockets

Power supplies

Xenon flash lamps modules

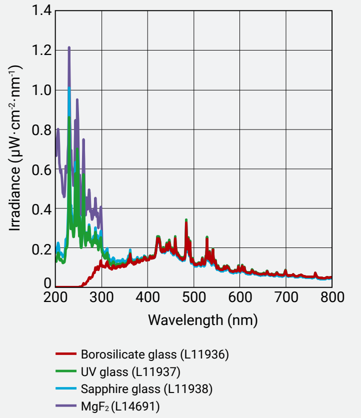
These devices are available as stand-alone emitters or modules with an integrated trigger socket and power supply for easy integration.

■ Spectral distribution (Typ.)
・UV region of 20 W xenon flash lamp



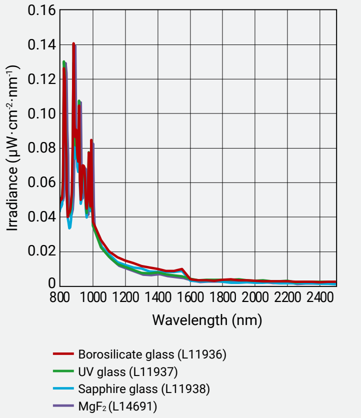
Measurement conditions
Under nitrogen atmosphere

■ Spectral distribution (Typ.)
・Visible region of 20 W xenon flash lamp



Measurement conditions
Main discharge voltage: 1000 V
Main discharge capacitance: 1.0 μF
Repetition rate: 40 Hz
Detector: Si photodiode
(200 nm to 800 nm, Spectral bandwidth 1 nm)
Measurement distance: 500 mm

■ Spectral distribution (Typ.)
・Infrared region of 20 W xenon flash lamp



Measurement conditions
Main discharge voltage: 1000 V
Main discharge capacitance: 1.0 μF
Repetition rate: 40 Hz
Detector: Si-InGaAs photodiode
(200 nm to 800 nm, Spectral bandwidth 1 nm)
InGaAs photodiode
(1600 nm to 2500 nm, Spectral bandwidth 5 nm)
Measurement distance: 500 mm

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Hamamatsu's Xenon Flash lamps feature instantaneous high peak output, a compact design, low heat generation and a continuous emission spectrum from 160 nm up to mid-infrared wavelengths making it the ideal light source for miniaturized instruments.

These lamps have a guaranteed lifetime of 10 billion flashes and offer output powers spanning from 2 W up to 60 W.

Conclusion

In conclusion, water quality monitoring has become increasingly important in environmental conservation and drinking water management. While traditional sampling programs provide only a partial understanding of water quality, UV-Vis spectroscopy offers real-time, accurate, and cost-effective measurements of various water parameters. Additionally, online UV-Vis spectrophotometers' performance can be improved by choosing the most suitable broadband light source. With advances in technology and increasing concerns about water quality, UV-Vis spectroscopy is expected to become an essential tool for water quality management.

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