

Review

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Review

Spectroscopy-Based Water Quality Analysis and Potential Applications in Livestock Farming

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Abstract

Water quality monitoring and evaluation are essential across multiple sectors, including public health, environmental protection, agriculture and livestock management, industrial processes, and broader sustainability efforts. Conventional water analysis techniques, although accurate, they are often constrained by the labor-intensive nature, extended processing times, and limited applicability for in-situ, real-time monitoring. In recent years, spectroscopy-based methods have gained prominence as alternatives for water quality assessment, particularly when combined with chemometric analyses and advanced technological systems. This review provides an overview of the current advancements of spectroscopy-based water monitoring, with a focus on spectroscopy techniques operating within the Ultraviolet/Visible (UV/Vis) and Infrared (IR) spectral regions, which are currently applied for the assessment of a broad range of physicochemical, and biological parameters relevant to livestock water management, including chemical oxygen demand (COD), dissolved organic carbon (DOC), nitrates, microbial contamination, and heavy metal ions. The findings highlight the growing utility of spectroscopy as a reliable tool in water quality monitoring and underpin for the need for continued research into scalable, sensor-integrated solutions tailored for use in livestock farming environments.

Keywords: water quality analysis; water quality parameters; spectroscopic methods; spectroscopy; chemometrics; machine learning; precision livestock farming

1. Introduction

Water is the most vital resource on Earth and indispensable for sustaining life. It occupies approximately 75% of the planet's surface [1] playing a crucial role in climate regulation and ecological balance. In the human body, it constitutes about 60-65% and serves biochemical reactions, thermoregulation and metabolic function [2]. Roughly 97% of the surface water is saline, leaving only 3% as freshwater available for consumption and other anthropogenic applications. However, merely 0.06% of this freshwater is contained in accessible reservoirs such as lakes and rivers, while the remaining 99.4% is found in subsurface aquifers, glaciers and wetland ecosystems showcasing the dependence on groundwater resources for potable and agricultural water supply[3].

The universal dependency of all life forms on Earth underscores the critical role of water in maintaining biological homeostasis and ecosystem stability. Nowadays, the One Health approach emphasizes the interdependence of human, animals', and environmental health and includes water safety as a basic component. Globally, institutions such as the World Health Organization (WHO),

the Centers for Disease Control and Prevention (CDC), and the World Organisation for Animal Health (WOAH) actively support integrative approaches to public health and environmental sustainability [4–6]. Recognizing the deep interconnections between various sectors including health, food safety, water resources and energy it becomes evident that effective prevention and risk mitigation strategies require interdisciplinary collaboration among professionals from medicine, veterinary science, chemistry, physics, environmental science, epidemiology, public health, and policy development. In this context, addressing the increasing challenge of improperly managed water resources and sanitation services remains a priority for billions of people worldwide. The Sustainable Development Goal (SDG) 6 emphasizes the necessity of sustainable management of water resources, wastewater treatment, and ecosystems preservation, while recognizing the significance of universal access to clean water for everyone by 2030.

Recent advancements across multiple production sectors, including industrial manufacturing, agriculture, and livestock farming, have resulted in various pollutants entering critical water sources, either directly, via seas, rivers, and lakes or indirectly through atmospheric deposition and soil infiltration impacting water quality and safety. Additionally, the rapid growth of industrial and agricultural production promptly affects the global water footprint [7], as vast amounts of water are consumed in the manufacturing of goods. For example, approximately 11,000 liters of water are needed to produce a liter of milk [8], while 15,400 liters are needed for a kilogram of boneless beef [9]. Except from the increasing demands for production, water contamination, excessive evaporation driven by climate change, and disruptions to the typical water cycle pattern further contribute to the water sources degradation and scarcity.

Various factors, including natural disasters, seasonal variations, and fluctuations in water availability, can lead to rapid or gradual changes in water quality with respect to its potability and in some cases its suitability for other applications [10]. The early detection of water quality fluctuations is of pivotal importance to secure the desirable water quality and safety status, enabling efficient responses to contamination events. Indeed, the increasing frequency of extreme weather events, such as heavy rainfall resulting in floods, and prolonged droughts causing water shortages, have a devastating impact on both water quality and availability.

Therefore, the need for sustainable water resource exploitation and advanced, real-time, *in-situ*, monitoring systems of water quality has emerged, with applications aiming to support evidence-based and sustainable water management strategies of surface and groundwater sources [11]. Spectroscopy has emerged as a versatile and efficient tool for water quality assessment across a wide range of applications. Spectroscopic techniques are extensively utilized in almost all technological and scientific domains [12], enabling the determination of the composition, structural properties, and physicochemical characteristics of materials and substances [13], applications of key importance for agriculture and livestock farming, where accurate and reliable monitoring of water quality is essential for optimizing productivity, reinforcing animal health and welfare, and maintaining sustainable resource management.

The objective of this review was to summarize and compile the available literature on spectroscopy for water quality assessment applications, with particular focus on contaminants that are commonly present in livestock farming environment. In particular, Ultraviolet/Visible (UV/Vis) and Infrared (IR) spectroscopy are mainly examined, with applications ranging from monitoring key water quality parameters, including chemical oxygen demand (COD), dissolved organic carbon (DOC), phosphorus, nitrates, and microbial contamination, across different types of water sources such as surface water, groundwater, wastewater, and drinking water supplies. Additionally, the performance, applicability, and adaptability of each spectroscopic method and applications thereof are discussed. Finally, the review explores chemometric techniques, discussing their contribution to improving data interpretation, accuracy, and predictive modeling in spectroscopic analyses of water quality.

2. Spectroscopy Principles

2.1 Spectroscopy

Spectroscopy is the study of the light absorbance and emission in relation to the wavelength of the radiation that a medium is exposed to. It measures and interprets electromagnetic spectra[12,14] based on the principle that the energy of light is inversely related to its wavelength (λ) as described by the Planck’s equation.

$$E = \frac{h \times c}{\lambda} \tag{1}$$

Where E is the energy of the light in J , h is the Planck's constant ($6.62 \times 10^{-34} J \times Hz^{-1}$), λ is the wavelength of the light in m and c is the speed of light ($\approx 3 \times 10^8 m/s$).

2.2 Electromagnetic Spectrum

The distribution of electromagnetic radiation by wavelength or frequency is known as the electromagnetic spectrum [15]. The term spectrum was first used by Isaac Newton in 1666 to refer to the multicolored band of light that appeared when he placed a glass prism in the path of a sunbeam [16]. Later, in 1800, William Herschel was researching the temperature of various colors when he discovered infrared radiation while passing a thermometer through prism-split light [17]. One year later, Johann Ritter noticed invisible rays beyond the violet end of the visible spectrum, that cause specific chemical reactions, he called them "chemical rays". This spectral region was given the name ultraviolet [18].

The electromagnetic spectrum consists of the whole range of electromagnetic radiation and includes many subranges, such as Visible (Vis) light in the region from 380 nm to 750 nm, Ultraviolet (UV) radiation in the region from 10 nm to 400 nm, and Infrared (IR) radiation in the region from 750 nm to 1 mm as illustrated Figure 1. Currently, the majority of frequencies and wavelengths of electromagnetic radiation are exploited in spectroscopic applications.

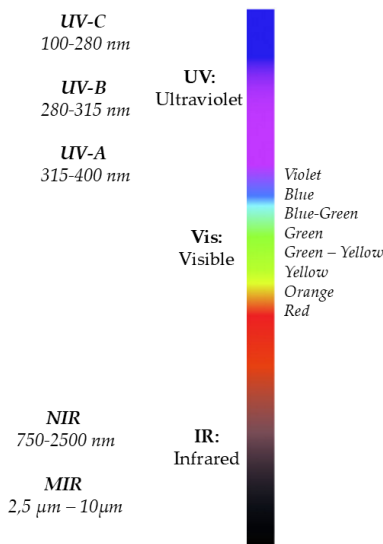


Figure 1. The electromagnetic spectrum and wavelength ranges of electromagnetic radiation applied in water quality analyses [19] (modified).

2.3 Lambert-Beer Law

The quantitative analysis of a range of substances' quality parameters using absorption spectra is based on the Lambert-Beer law [20,21]. An illuminated medium partially absorbs the light energy that irradiates its surface, allowing a weakened intensity to pass through it. This phenomenon is governed by Lambert-Beer’s law [22] and the following mathematical expression:

$$A = \log_{10} \left(\frac{I_0}{I} \right) = \log_{10} \left(\frac{1}{T} \right) = \epsilon \times d \times c \quad (2)$$

In equation (2) the absorbance (A) is proportional to the product of the optical path length (d) in (cm) and the analyte’s concentration (c) in (mol/L); (ε) is the molar absorptivity in (L/(mol * cm)), and inversely proportional to the transmittance (T). In Figure 2 a schematic representation is shown.

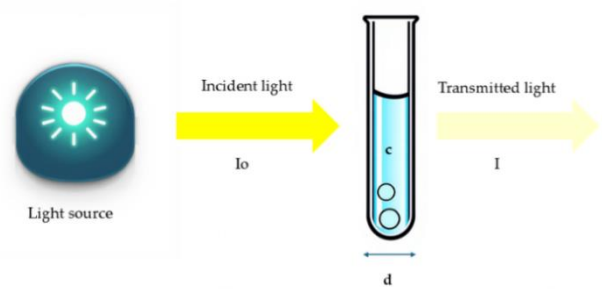


Figure 2. Schematic representation of Lambert-Beer’s law.

3. Water Quality and Its Importance in Livestock Farming

Chemical contamination of water is a challenging issue of major concern with the potential detrimental immediate and long-term effects on ecosystems and public health [23]. Water resources are broadly classified into surface water and groundwater distinguished by their origin [24]. Water pollution occurs in both categories due to a variety of anthropogenic factors associated with industrial discharge, agricultural runoff, and waste from livestock operations.

Livestock farming and animal-derived product industry account for nearly one-third of the global agricultural water consumed, highlighting their substantial demand for freshwater resources [25]. Livestock sector alone consumes approximately 10% of the estimated annual global water flows [26], while the quality standards of potable water are similar in both animals and humans [27]. Nevertheless, in many cases, the source of water in livestock farms may vary significantly. Table 1 summarizes the acceptable thresholds of different analytes in the water used for animal watering and irrigation in the USA. The variation between the two thresholds is evidenced, despite irrigation water being widely used in animal watering.

Table 1 Water quality thresholds for animal watering and crop irrigation in the USA [27].

Elements	Threshold for animal watering	Threshold for crop irrigation
chlorine (ppm)	300	
chromium (ppm)	1.0	1.0
copper (ppm)	0.5	5.0
lead (ppm)	0.1	10.0
mercury (ppm)	0.01	
nickel (ppm)	1.0	2.0
nitrate nitrogen (ppm)	100	
pH	8.5	
phosphorus (ppm)	0.7	
sulphates (ppm)	300	
total bacteria (n/100 ml)	1000	
total dissolved solids (ppm)	5000	

ppm: parts per million, n: numbers

Some water sources other than tap water utilized to cover farm animal water demands include i) wells, ii) rivers, ponds, lakes and other surface water spots, and iii) boreholes constructed for water extraction, providing a reliable alternative in areas with limited surface water availability.

The livestock sector needs a substantial quantity of water to support the increasing production demands and has a considerable impact on water resources quality and hygiene [28]. The excessive manure and overall livestock-related waste production that affects water quality has resulted by the intensification of livestock farming, also known as the "livestock revolution" [29]. Particularly in intensively reared animals, mineral and protein supplementation frequently surpass the animals' nutritional requirements, leading to nutrient-rich manure. While this can be beneficial for agriculture, it also poses environmental risks. Excess nitrogen and phosphorus from manure can seep into groundwater and flow into surface waters, contributing to water contamination [30–32].

Additionally, manure application introduces heavy metals like copper and zinc which accumulate in soils and enter the aquifer and the food chain [33]. Moreover, fertilizers, pesticides, and other agrochemicals in agricultural production introduce relevant residues and pollutants into water bodies [34]. Finally, antibiotics used in livestock prophylaxis and metaphylaxis further contribute to water pollution, as 30–90% of them are excreted unmetabolized into the environment facilitating antimicrobial resistance within the ecosystems [35].

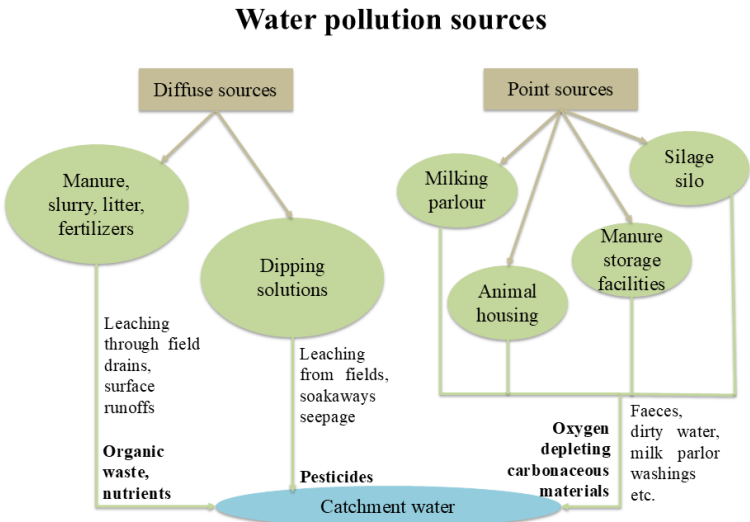


Figure 3. Diffuse and source point paths of different pollutants in catchment water in livestock farming areas (modified) [31].

There are multiple sources of water contamination in livestock farms making it increasingly important to efficiently assess the quality and safety of the water consumed by animals.

3.1 Water Quality Parameters and Standards

Water quality is defined by a variety of characteristics which determine its suitability for different purposes. Water is classified in four categories according to its quality, namely, potable, palatable, polluted, and infected water (Figure 4) [24].

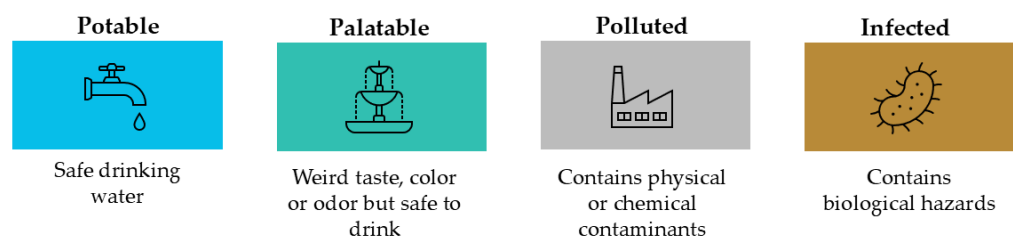


Figure 4. The four water quality categories.

Various parameters are essential for the comprehensive assessment of water quality [36]. These parameters are typically classified into three main groups: physical, chemical, and biological as outlined in Table 2 [37]. The presence of extraneous substances in water, which do not inherently pose a health risk, such as sediments, color, or taste-altering compounds, is described as water contamination [38]. In contrast, water pollution denotes contamination that adversely affects the suitability of water for specific uses, resulted from anthropogenic activities [39].

Table 2. Physical, chemical, and biological parameters used to define water quality [24].

Physical	Chemical	Biological
turbidity	pH	bacteria
temperature	acidity	algae
color	alkalinity	viruses
taste and odor	chloride	protozoa
solids	chloride residual	
electrical conductivity (EC)	sulfate	
	fluoride	
	iron and manganese	
	copper and zinc	
	hardness	
	dissolved oxygen	
	biochemical oxygen demand (BOD)	
	chemical oxygen demand (COD)	
	toxic inorganic substances	
	toxic organic substances	
	radioactive substances	

Physical parameters refer to the observable properties of the water such as temperature, turbidity, color, electrical conductivity, and total suspended solids. Physical parameters of the water influence its appearance and its capacity to carry or dissolve other substances, while excessive turbidity or temperature fluctuations can reduce water intake in farm animals impairing their welfare, productivity and thermoregulation efficiency.

Chemical parameters refer to inorganic and organic compounds, including pH, dissolved oxygen, nitrates, phosphates, heavy metals (e.g., lead, arsenic), and salinity. These elements affect the metabolic functions of animals, with contaminants like nitrates or abnormal pH levels potentially causing toxicity or reduced productivity. Some of the chemical parameters are explained below:

- Chemical oxygen demand (COD) is defined as the quantity of oxidants consumed by the reducing substances in an one-liter oxidized water sample under specific conditions, expressed in milligrams per liter. It demonstrates the level of contamination brought on by introducing reducing agents into water [21].

- Dissolved organic carbon (DOC) is representing a universal element of the freshwater carbon cycle. It is a water disinfection byproduct that affects human health and can impair the effectiveness of aquatic ecosystems and weaken ultraviolet radiation [40].
- Nitrogen and phosphorus-containing compounds (e.g., detergents, fertilizers) are being released into the aquifer in mass quantities, disrupting the nitrogen and phosphorus equilibrium in aquatic ecosystems and causing eutrophication, the rapid and excessive growth of algae and other microorganisms, and the aquatic ecosystem degradation due to hypoxia. Consequently, water quality will eventually deteriorate and aquatic life will be challenged, which will have a remarkable impact on marine ecosystems and human production activities. [21].

The permissible limits for the aforementioned water quality parameters are variable and contingent upon factors, including the intended application of the water (e.g., drinking, agricultural irrigation, industrial use), as well as the regulatory framework established by individual countries or international organizations [37]. Drinking quality indicators and the thresholds of various relevant analytes in Europe and as proposed by the WHO are presented in Table 3.

Table 3. Indicative parameters for drinking water quality and associated limits [37].

Parameter	Europe [41]	WHO [42]
pH	6.5-9.5	-
Electrical conductivity ($\mu\text{S cm}^{-1}$ at 20 °C)	2500	-
ammonia/ammonium (mg/l)	0.5	0.2
chloride (mg/l)	250	250
chromium ($\mu\text{g/l}$)	25	50
copper (mg/l)	2.0	2.0
fluoride (mg/l)	1.5	1.5
lead ($\mu\text{g/l}$)	5.0	10
nitrate (mg/l)	50	50
nitrite (mg/l)	0.5	3.0
sulphate (mg/l)	250	-
pesticides (total) ($\mu\text{g/l}$)	0.5	-

Biological parameters refer to the presence of microorganisms such as bacteria, viruses, protozoa, and algae, with some of them being critical in livestock systems due to their association with waterborne infections and related diseases.

Waterborne diseases arise when pathogens are transmitted through the consumption of contaminated water. Water contamination primarily occurs via fecal pollution, with enteric bacteria such as *Escherichia coli* serving as key indicators of fecal presence; however, their detection alone does not suffice for assessing water safety. Moreover, environmental factors such as rising water temperature, flooding, and extreme weather events exacerbate the risk of pathogens' survival and transmission, increasing the likelihood of disease outbreaks in both animals and humans [23]. Indeed, diarrheal diseases - often caused by waterborne pathogens - are responsible for 1.8 million deaths annually, particularly among children in developing countries. Some of the most common waterborne pathogens include *Vibrio cholerae* (Cholera), *Shigella spp.* (Dysentery), *Salmonella spp.* (Typhoid) [43].

The integration of spectroscopy-based spectrum acquisition with machine learning-based analytical techniques has emerged as an increasingly popular approach for the detection of pathogens in the water. A representative example is the study by Feng et al. [44], in which the UV/Vis spectra were captured for samples contaminated with bacteria species such as *E. coli* and *Salmonella typhi*, while artificial neural networks were used to build classification models enabling the automated pathogen identification based on distinct spectral features.

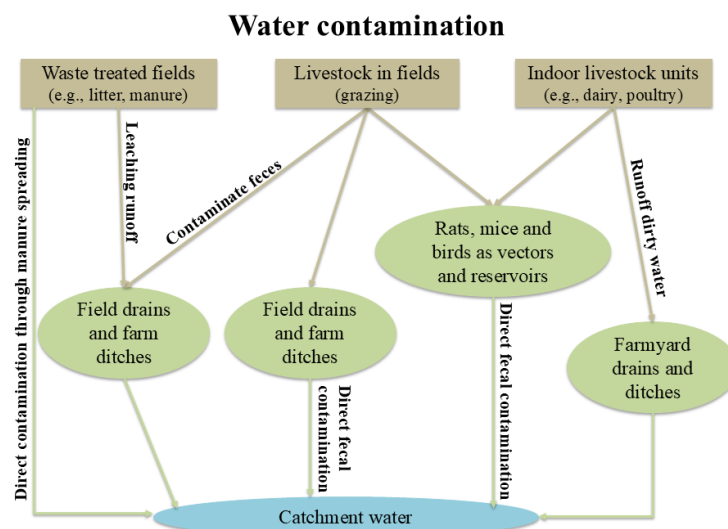


Figure 5 Paths of catchment water contamination with microbial and protozoan micro-organisms in livestock farming areas (modified) [31].

4. Chemometrics

Spectroscopic techniques and chemometrics are harmoniously and effectively combined in water quality analysis. Chemometrics refer to a broad range of statistical methods utilized to analyze chemical data, as well as to data mining techniques and machine learning (ML) algorithms. Based on the occurrence of data labeling, chemometric methods are divided into supervised and unsupervised methods. Supervised chemometric methods are applied either on classification problems of items assigned to discrete categories or on regression problems where the input data are associated with a continuous variable. Contrarily, unsupervised learning builds on uncovering typical patterns or structures in data sets without external labeling input. Unsupervised learning is commonly employed during the initial stages of analysis to reduce the dimensionality of datasets, ensuring that only the most meaningful and informative data are kept for further processing.

One of the most widely used unsupervised learning algorithms is Principal Component Analysis (PCA), which reduces a large dataset of intercorrelated variables to a smaller dataset, while explaining the largest variance of the dataset through newly established independent variables known as principal components [45].

The most popular supervised chemometric algorithms used in water analysis applications are:

- Partial Least Squares (PLS): It is a regression model that predicts a group of dependent variables from a group of independent variables (predictors). By projecting both input and output variables into a new space which maximizes the covariance allowing to model the interactions between them, it is considered efficient when there are more predictors than observations or in cases of multicollinearity [46].
- Support Vector Machines (SVM): They are supervised learning models, considered as binary linear classifiers that classify observations by finding the optimal boundary which maximizes the distance (margin) between different classes [47]. Using various kernel functions, they are effective in high-dimensional issues and perform well on both linear and non-linear classification tasks.
- Artificial Neural Networks (ANNs): ANNs are computational models based on a network that consists of several connected nodes inspired by the human brain which are known as artificial neurons, with the simplest one being *perceptron* (used for binary classification of linearly separable data) [48]. There are many types of NNs specialized in different scientific areas and applications including spatial data and image-like pattern analyses (Convolutional NNs) [49].

- Decision Trees (DT): It is a tree-like non-parametric method that can be used to solve classification and regression problems. The leaves of the trees represent different labels or outcomes (classes). They are easy to implement however, in the case of complex datasets they are sensitive to overfitting [50].
- Random Forest (RF): is considered an ensemble learning method for which multiple DTs are trained. For classification problems, the model outputs the class chosen by the majority of trees, while for regression problems, it returns the average of the trees' outputs [51].

There are numerous studies assessing the performance of ML algorithms in water quality analysis (Table 4, 5). In one of them, Zhu et al. [52] reviewed various ML methods across different aquatic environments (groundwater, drinking water, wastewater, and marine environments), with Support Vector Machines (SVM) and Artificial Neural Networks showing the best performance. In other studies, various ML algorithms were evaluated based on their efficiency when used either in water quality classification or in prediction applications. Specifically, Nasir et al. [53] studied numerous different classifiers, such as RF, DT, and SVM on a dataset derived from the analysis of 1679 water samples and found that the CATBoost algorithm achieved the highest accuracy for the prediction of the studied water quality parameters. Similarly, in the study by Kaddoura [54] the aim was to evaluate different ML algorithms for the prediction of water quality, with eleven algorithms being tested; based on the F1 scores and the ROC curve values, SVM and k-nearest neighbor (k-nn) algorithms were found to perform better. Finally, Najah Ahmed et al. [55] also investigated the use of ML methods with Adaptive Neuro-Fuzzy Inference System (ANFIS), Radial Basis Function Neural Networks (RBF-ANN), and Multi-Layer Perceptron Neural Networks (MLP-ANN) being exploited to improve the prediction capacity of water quality.

5. Water Quality Analysis Applications

Spectroscopy has a wide range of applications in water quality analysis across various aquatic systems including surface water, groundwater, and wastewater [34,56,57]. Herein, we present different applications in these aquatic systems; however, it is important to note that spectroscopic methods also play a significant role in water quality assessment for fish farming and in the analysis of water content in soil [58,59]. Spectroscopic techniques such as NIR spectroscopy, and UV/Vis spectroscopy, are primarily employed in evaluating livestock water resources, facilitating the detection of analytes and specific contaminants, and assessing the quality of valuable water resources. A key advantage of these methods is their ability to enable real-time, on-site analysis, in contrast to conventional water quality assessment techniques, which are time-consuming and typically conducted in specialized laboratories.

A typical spectroscopical water analysis set-up is demonstrated in Figure 6. Using the appropriate spectroscopic method, spectral data are collected, analyzed, and combined with a variety of chemometric techniques to acquire the desirable results for water quality.

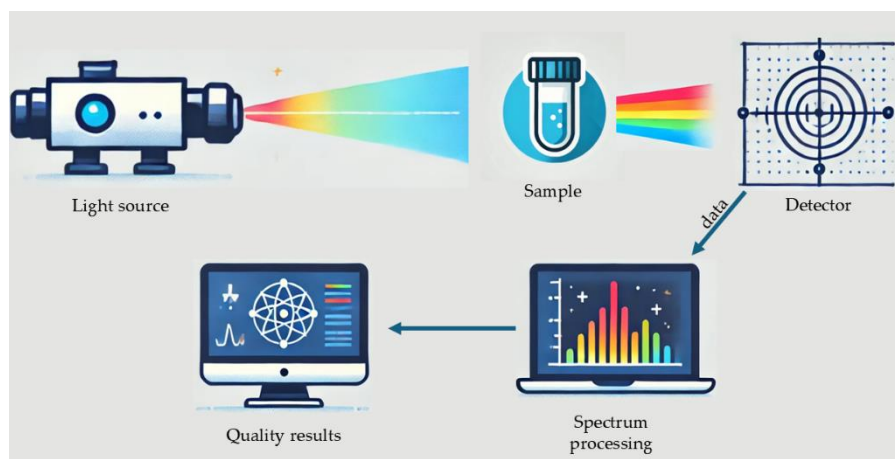


Figure 6. Schematic representation of the spectroscopic analysis process in the water quality assessment.

5.1 Ultraviolet-Visible (UV/Vis) Spectroscopy

Ultraviolet-Visible spectroscopy is a low-cost spectroscopic method that can efficiently and accurately detect and identify a variety of physical, chemical, and microbiological water quality parameters [20]; it is currently utilized for a variety of water analyses applications extending from bacterial or contamination detection to Dissolved organic carbon (DOC) quantification as summarized in Table 4.

Feng et al. [60] used a UV/Vis spectrophotometer to acquire the spectra of water samples contaminated by bacteria at 200-900 nm; for the characterization of samples, principal component analysis-Monte Carlo (PCA-MC) was used to separate the spectrum of mixed-bacteria contaminated water samples and measure the microbial content. The method succeeded to efficiently monitor water microbial content achieving a 0.9954 coefficient of determination (R^2) in the testing set. Similarly, several studies have applied UV/Vis spectroscopy combined with chemometric tools for the monitoring of chemical oxygen demand (COD). Chen et al. [61] monitored (COD) in wastewater using UV/Vis spectroscopy combined with partial least squares (PLS); measuring the spectra of 82 samples with wavelength ranging from 200 to 650 nm for different wavelength paths they generated a slope-derived spectrum achieving a coefficient of determination (R^2) equal to 0.936. The combination of UV/Vis spectroscopy with PLS to measure COD was also used by Li et al. [62]; specifically, the best prediction performance was acquired using synergy interval PLS (siPLS) with correlation coefficient of prediction (R_{pred}) of 0.8334 and root mean square error of prediction (RMSEP) of 2.63. Diffuse reflectance UV/Vis spectroscopy and PLS were also used by Agustsson et al. [63] to assess COD and turbidity in water, achieving R^2 values equal to 0.85 and 0.96, respectively, between the reference and the measured concentrations. Further advancing COD analysis, Hu et al. [64] measured COD by compensating the impact of turbidity in the spectral measurements acquired using UV/Vis spectroscopy. The method reached 0.99 R^2 and 2.42 mg/L root mean square error (RMSE). Moreover, in another study, Hu et al. [65] used UV/Vis spectrum for the detection of eight typical contaminants and proposed four surrogate parameters for rapid prediction of the contaminants' category.

The applications of UV/Vis spectroscopy have also been extended to natural water bodies, demonstrating the potential for real-time, field monitoring. Zhu et al. [66], used a portable UV/Vis spectrophotometer (spectro:lyser, S:CAN Messtechnik GmbH, Austria) for the quantification of DOC and iron (Fe) in river water samples originated from northern Europe. They acquired in-situ and ex-situ spectral data, and exploited three different analysis models, namely, PLS, principal component regression (PCR) and multiple stepwise regression (MSR). For both DOC and Fe, the MSR model proved to be the most efficient one, reaching R^2 values of 0.971 and 0.989 respectively. Similarly, Cook et al. [67] studied DOC in tropical peatlands, achieving validation R^2 values that ranged from 0.86 to 0.93.

The classification of drainage water into four different categories (domestic sewage, mixed rainwater, rainwater, and industrial sewage) using the UV/Vis spectral data and neural networks (NN) algorithms was studied by Zhu et al. [68], achieving an overall sensitivity of 97.9% and specificity of 99.3% with the application of convolutional NN (CNN). In the study by Wang et al. [69], the goal was to detect in real-time contamination events in the water distribution system with UV/Vis spectrometry and Bayesian analysis for event classification; for contamination events with concentrations above 30 $\mu\text{g/l}$, the results were satisfying, though further work was deemed necessary to improve and broaden the applicability of the proposed method.

Finally, UV/Vis spectroscopy has also proven effective for quantifying a variety of analytes in different aquatic environments. In the study by Etheridge et al. [70], the concentration of nitrogen, carbon, phosphorus and suspended solids in tidal marsh was investigated, among other parameters; combining UV/Vis absorption spectrum with different calibration models, depending on the parameter, they achieved R^2 values ranging from 0.750 to 0.995. Furthermore, UV/Vis spectroscopy

was also employed by Mason et al. [71] in their work to detect and quantify residues of the antibiotics lincomycin and tylosin.

Table 4. Ultraviolet-Visible spectroscopy (UV/Vis) applications and performance.

Wavelength (nm)	No of samples	Origin of sample	Chemometri cs	Application	R ²	RMSE	Referen ce
200 – 900	11	cultivated bacteria	PCA-MC	bacteria detection	0.9954	-	[60]
220 – 750	66	fabricated	PLS	COD, turbidity	0.99	2.42 mg/L	[64]
200 – 1100	25	wastewater	-	organic contaminant detection	-	-	[65]
270, 350	252	tropical peatlands	NLR, LR	DOC quantification	0.86 – 0.98	1.51 - 6.89 mg/L	[67]
200 – 800	183, 142	catchment s water	MSR	DOC, Fe	0.973, 0.989	2.599 mg/L, 108.905 µg/L	[66]
193.91 – 1121.69	144	lake water	siPLS	COD	0.8334	2.63 ¹	[62]
200 – 650	98	wastewater	FiPLS	COD	0.936	122 mg/L ²	[61]
200 – 1100	48	fabricated	PLS	COD, turbidity	0.69, 0.95	35%, 21% ³	[63]
220 – 700 *	192	different sewer networks	FNN, CNN	drainage type recognition	-	-	[68]
225 – 260 260 – 320 320 – 700	144	fabricated	PLS	nitrate, COD, turbidity	0.993, 0.982, 0.998	1.29 mg/L, 2.337 mg/L, 0.696 mg/L	[72]
250 – 600	ND	fabricated	EKF-DM	copper, cobalt, nickel	0.9958, 0.9976, 0.9915	-	[73]
520 / 610 **	ND	fabricated	ND	metal ions	-	-	[74]

RMSE: Root Mean Square Error, PCA: Principal Component Analysis, MC: Monte Carlo, PLS: Partial Least Squares, COD: Chemical Oxygen Demand, NLR: Non-Linear Regression, LR: Linear Regression, DOC: Dissolved Organic Carbon, MSR: Multiple Stepwise Regression, siPLS: synergy interval Partial Least Squares, ^{1,2}RMSEP: Root Mean Square Error of Prediction, FiPLS: Forward interval Partial Least Squares, ³SEP: Standard Error of Prediction, FNN: Fully connected Neural Network, CNN: Convolutional Neural Network, EKF-DM: Extended Kalman Filter and Derivative Method *sensitivity (%): 95.8, 97.8, specificity (%): 98.6, 99.3, **Limit of Detection: 30 parts per billion for lead ions and 89 parts per billion for aluminum ions, ND: Not Defined

5.2 Infrared Spectroscopy

Infrared (IR) spectroscopy has emerged as a rapid spectroscopic analytical technique with high precision and a plethora of applications [20]. In water analysis, its range of application extends from measuring key water quality parameters such as COD and alkalinity [75] to detecting various analytes including heavy metals [76] (Table 5). Infrared spectroscopy encompasses several techniques including Near-Infrared Spectroscopy (NIRS), Mid-Infrared Spectroscopy (MIRS), and Fourier Transform Infrared Spectroscopy (FTIR). The main distinction between NIRS, MIRS, and FTIR lies in their operational wavelength ranges, with NIRS operating in the range of 750 to 2500 nm, MIRS from

2.5 to 10 μm , while FTIR typically operates within the MIR region, but in some cases extends into the NIR and the Far-Infrared (FIR) regions.

The absorbance spectrum of 83 polluted samples was collected using a NIR spectrophotometer (NIRSystems 5000, produced by Foss, Denmark) in the study by Chen et al. [77]. The aim was the rapid evaluation of water pollution in agricultural applications. To this end, a CNN was designed and trained to enhance the prediction accuracy of NIR spectroscopy, attaining a calibration correlation coefficient R_c of 0.938 and reducing the RMSE of calibration to 19.86 mg/L. In another study by Chen et al. [57], focusing on water pollution assessment, the prediction of the samples' COD values was performed using a least square support vector machine (LSSVM) algorithm. The optimal results (RMSECV = 20.19 mg/L) were obtained using a 5-fold cross-validation LSSVM model, with 5 hidden layers and 12 neurons per layer, enhanced with logistic-based kernel function. Pollution detection via NIRS was also investigated by Xu et al. [34], where they successfully distinguished polluted from non-polluted samples. Similarly, in a study by Skou et al. [78] the combination of NIRS and PLS was applied to monitor water quality in dairy processing units. In particular, they focused on urea content, a compound with potential biological risk, and achieved a RMSEP of 12.1 ppm concerning the process model validation. Bacterial identification was the focus of studies by Alexandrakakis et al. [79] and Cámara-Martos et al. [80], both employing NIRS alongside multivariate analysis. Alexandrakakis et al. suspended bacteria in water, and collected NIR spectra from aqueous solutions, achieving classification accuracies ranging from 77.4% to 100.0% using different chemometrics methods. Cámara-Martos et al. utilized FT-NIR, demonstrating successful quantification at high bacterial concentrations (3-9 log cfu/mL), with R values between 0.98 and 0.99. The quantification of pharmaceutical compounds, such as ibuprofen (IBU), sulfamethoxazole (SMX) and β -estradiol (E_2) in wastewater using FT-NIR spectroscopy was investigated by Quintelas et al. [81], yielding promising results with R^2 values ranging from 0.858 to 0.963 across the studied compounds.

The application of FTIR-ATR (attenuated total reflectance) spectroscopy to urban water bodies was investigated by Wu et al. [82] and Zheng et al. [83] focusing on nitrate and phosphorus concentrations, respectively. Fourier Transform Infrared is used as a biochemical fingerprint technique [84], while ATR serves as a sampling method used alongside with FTIR, allowing solid and liquid samples to be placed directly onto a crystal surface, with minimal preparation, where infrared light is directed onto them [85,86]. In another study, Wu et al. [82] reported R^2 values ranging from 0.889 to 0.972, depending on the sampling month, and R^2 values ranging from 0.784 to 0.994 across different nitrate concentrations. Regarding phosphorus monitoring, Zheng et al.[83] found that integrating FTIR-ATR with machine learning techniques was highly effective; indeed, self-adaptive PLS model yielded the most promising results with $R^2= 0.973$ and $RMSE_v=0.015$ mg/L.

Table 5. Infrared spectroscopy applications and performance in water analysis.

Wavelength	No of samples	Origin of sample	Chemometrics	Application	R^2	RMSE	Reference
200 – 14000 cm^{-1}	276	sludge wastewater treatment	PCA, PLS	IBU,	0.943,	5.47 %,	[81]
				SMX,	0.948,	4.91 %,	
				E_2 ,	0.951,	6.16 %,	
				EE_2 ,	0.858,	10.12%,	
				CRB	0.963	5.10 %	
4000 – 650 cm^{-1}	94	river and lake water	PCA, PLSR	nitrate monitoring	0.8868 – 0.9720,	-	[82]
					0.7836 – 0.9938		
4000 – 800 cm^{-1}	100	river and lake water	PCA, SA-PLS	phosphorus monitoring	0.973	0.015 mg/L	[83]

390 – 1000 nm	ND	lake water	-	polluted/ non polluted	-	-	[34]
780 – 2500 nm	83	industrial wastewater	CNN	pollution level	0.914	25.47 ¹	[77]
780 – 2500 nm	83	wastewater	LSSVM	COD	0.912	20.19 mg/L*	[57]
700 – 900 nm *	418	cultivated bacteria	PCA, PLS2-DA, SIMCA	bacterial identification	-	-	[79]
1100 – 2500 nm	140	cultivated bacteria	PCA, PLS	bacterial identification	0.983 – 0.99	0.09 – 0.28 log cfu/mL	[80]
700 – 2500 nm	32	dairy process	PLS	urea, lactose		12.1 ppm	[78]

RMSE: Root Mean Square Error, PCA: Principal Component Analysis, PLS: Partial Least Squares, IBU: ibuprofen, SMX: sulfamethoxazole, E2: β -estradiol, EE2: ethinylestradiol, CRB: carbamazepine, PLSR: Partial Least Squares Regression, SA-PLS: Self-adaptive Partial Least Squares, CNN: Convolutional Neural Network, ¹: RMSEC: Root Mean Square Error of Calibration, COD: Chemical Oxygen Demand, ND: Not Defined, LSSVM: Least Squares Support Vector Machine,*accuracy (%): 77.4 – 100, PLS2-DA: Partial Least Squares Discriminant Analysis, SIMCA: Soft Independent Modeling of Class Analogy

5.3 Other Spectroscopy Methods

Over the years, various methods have been studied for water analysis. Some of the studies have focused on water quality monitoring, addressing either instrumentation or application aspects [87–89], while others have investigated numerous techniques from a biosensor perspective, emphasizing the analytes detected [90]. Collectively, these studies illustrate the advancing landscape of analytical technologies in environmental monitoring and, more specifically, water quality assessment.

A combination of Raman scattering and Laser Induced Breakdown Spectroscopy (LIBS) was utilized by Liao et al. [91] for bacterial detection, achieving a linear detection range from 5×10^3 to 5×10^7 CFU/mL, with recovery values between 81.0% and 101.7%. In the study by Meng et al. [92], LIBS was applied in on-line/on-site water analysis for heavy metal detection. While aluminum enrichment resulted in a good limit of detection, the method was time consuming and unsuitable for real-time monitoring. In contrast, graphite enrichment proved more efficient in practical applications. Zhang et al. [56] employed fluorescence spectroscopy to identify water pollution originating from livestock farming. By integrating fluorescence measurements with multivariate statistical methods, the characteristics of dissolved organic matter (DOM) in groundwater were examined; their findings demonstrated that fluorescence-based techniques are effective for water pollution assessment, as hierarchical cluster analysis successfully classified samples into three distinct clusters based on varying degrees of contamination.

6. Future Research

Further development, specialization and validation of spectroscopic technologies for water analysis applications are still needed to overcome operational challenges, while improving their reliability under real-world conditions.

One of the main challenges is the use of portable or handheld instruments to obtain real-time water analysis results, either with respect to pollutant concentration measurement or to microbial/bacterial detection. Several studies have focused on this direction, employing different methods, such as LIBS or fluorescence spectroscopy for on-site analysis [11,92], however, further research is still needed to conclude their performance. Other spectroscopic methods with a proven analytical potential, should be further explored for the water analysis, such as Quantum Cascade Lasers (QCLs), which have demonstrated great promise in detecting ammonia in water [93].

Quantum cascade lasers are advantageous as a light source due to their adjustable energy bandgap engineering, which enables the design and production of lasers with highly specific emission spectra in the MIR and Terahertz (THz) regions. Additionally, the integration of QCLs into photonic integrated circuits (PIC) presents an attractive solution offering resilience, a compact device footprint, and the potential for low-cost production [94]. Considering these advantages, QCLs should be a key focus of future investigations in the field of water analysis.

An important direction that should be prioritized in future research is the implementation of ensemble methods wherein multiple algorithms will be combined to enhance prediction accuracy, rather than relying to a single algorithm. A similar approach could also be applied to spectroscopic techniques, where the fusion of multiple methods could yield more robust analytical capabilities.

Finally, another highly promising direction in water analysis is the combination of spectral analyses with other emerging digital technologies such as Internet of Things (IoT), cloud computing, remote sensing, blockchain, satellite imaging, etc. These technologies have the potential to significantly enhance spectroscopic methods through real-time monitoring, data fusion, and secure data management [95]. For instance, IoT sensors and cloud platforms can facilitate continuous analysis and instantaneous processing, while blockchain technology can provide data integrity and traceability [96]. Integrating these technologies with spectroscopic water analysis methods could lead to smarter, faster, and more reliable water quality assessment systems.

7. Conclusions

Based on the reviewed studies, spectroscopy-based methods appear as some of the most advanced tools for water quality evaluation. Their fast, non-invasive, and sensitive nature makes them ideal for environmental monitoring, especially in real-time conditions. Techniques like IR and UV-Vis spectroscopy have demonstrated robust performance across diverse aquatic environments (such as surface, drinking, or industrial water sources). When combined with chemometric modeling, these methods exhibit enhanced precision and strong predictive potential for the classification, forecasting, and continuous monitoring of key quality parameters.

The exploration of ensemble learning techniques and hybrid AI models should be further explored to more effectively leverage the strengths of spectroscopic data and chemometric tools. Moreover, the fusion of spectroscopy with emerging digital technologies, such as the IoT, cloud computing, and blockchain, could facilitate the development of automated, tamper-proof systems that enable real-time diagnostics, remote monitoring, and secure data traceability. Despite the promising results, real-world implementation of spectroscopic methods for water analysis remains limited in the livestock sector, showcasing a pressing need for field-scale validation and deployment of relevant technologies and for a relevant and updated regulatory framework. In any case, targeted applications should be prioritized in sectors like livestock farming, emphasizing on the detection of contaminants and pathogens of high relevance to animal health and food safety, utilizing sustained collaboration across disciplines—including analytical chemistry, data science, engineering, and agricultural sciences—to ensure these technologies are both scalable and sustainable.

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