

Conceptual Validation of a Near-Infrared Multi-Wavelength Scattering-Absorption Hybrid Sensor for Water Quality Monitoring

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 Cite This: *J. Sens. Sci. Technol.* Vol. 35, No. 5 (2026) 510-517

 <https://doi.org/10.46670/JSST.2026.35.5.510>

ABSTRACT: This study proposes a near-infrared multi-wavelength scattering-absorption hybrid sensor for integrated water quality monitoring. The sensor is specifically designed to discriminate air bubbles from suspended particles, which represent a major source of error in optical turbidity measurements. Three wavelengths are employed for distinct purposes: 850 nm for turbidity measurements in accordance with ISO 7027, 1450 nm for the detection of bubbles by exploiting the strong absorption band of water, and 660 nm as a reference channel to compensate for light source fluctuations and optical-window fouling. A sample/reference ratiometric dual-detector architecture was adopted for real-time error compensation. Proof-of-concept validation was performed using an extended Beer–Lambert model with literature-derived optical constants, under separately controlled scenarios in which particles and bubbles were considered independently. The discrimination index, $R = S(1450) / S(850)$, remained close to unity for pure water and particle-containing water, whereas it increased to above 5 under bubble-containing conditions with void fractions of 5–30%. A single threshold of $R_{th} = 2.0$, whose selection basis and sensitivity are discussed in this paper, successfully classified the three separately simulated conditions with an accuracy of 98% or higher. It should be emphasized that this result represents a proof-of-concept obtained from simulation rather than a measured sensor performance, and that particle-bubble coexistence conditions have not been evaluated here. This work corresponds to the concept-design stage; prototype fabrication and field validation across diverse water industry applications, including particle-bubble coexistence conditions, will be conducted in follow-up studies.

KEYWORDS: Multi-wavelength optical sensor, Near-infrared spectroscopy, Turbidity, Bubble discrimination, Ratiometric detection, Water industry monitoring

1. INTRODUCTION

As social and industrial demands for water safety and process control continue to intensify, the importance of real-time water quality monitoring is increasing across the water industry, including drinking-water treatment plants, wastewater treatment facilities, food and beverage process water, semiconductor and pharmaceutical ultrapure water, water reuse systems, and seawater desalination plants [1,2]. Optical turbidity sensors, which enable reagent-free, non-destructive, and real-time measurements, have therefore been

widely deployed in these applications [3]. The international standard ISO 7027-1:2016 specifies a scattering-based measurement method using a near-infrared light source (860 ± 60 nm) and a 90° scattering angle [4,5], and most commercial inline turbidimeters comply with this standard.

However, single-wavelength scattering methods have a fundamental limitation: they cannot distinguish air bubbles from suspended particles, because both produce similar optical scattering signals [6,7]. As summarized in Table 1, bubbles originate from different sources across water-industry sectors, but can generate spurious scattering signals in turbidity sensors. In particular, ozone contact and coagulation mixing in water treatment plants, aeration tanks in wastewater treatment facilities, bottling and pump cavitation in food and beverage processes, pressure fluctuations in industrial water piping, and pressure differences across RO/MF membranes in membrane-separation systems can introduce fine bubbles into the flow [8].

Under such bubble-prone conditions, frequent false alarms

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Received : Aug. 7, 2026, Revised : Aug. 23, 2026, Accepted : Aug. 28, 2026

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Table 1. Water quality monitoring requirements and typical bubble sources in each water industry application.

Application	Key water quality parameters	Typical bubble sources
Water treatment plant	Turbidity, color, organic matter	Ozone contact, coagulation and stirring
Wastewater treatment	Turbidity, suspended solids	Aeration and reaction tanks
Food and beverage process water	Turbidity, organic matter	Bottling, pump cavitation
Industrial water (semiconductor, pharmaceutical)	Ultrapure-water particles	Pipeline pressure fluctuations
Reuse and seawater desalination	Turbidity upstream of membranes	Pressure differences across RO/MF membranes

may lead operators to routinely disregard the sensor outputs – a phenomenon known as the “Wolf effect” – thereby delaying responses to actual water quality incidents occurs [9]. This problem is not confined to a specific application but is commonly encountered in optical water quality monitoring; therefore, a broadly applicable solution is required across different sectors of the water industry.

Various approaches have been proposed to address this issue. Representative examples include multi-angle scattering measurements based on the ratio of backscattering to forward scattering [10,11], time-domain spike filtering [8], and mechanical de-bubbling as a pre-treatment. However, multi-angle configurations require complex optical alignment and offer limited temporal resolution, time-domain filtering carries the risk of misclassifying signals from low concentrations of suspended particles as bubbles, and mechanical de-bubbling is difficult to implement in inline installations. Ultraviolet absorption at 254 nm is widely used as an indicator of aromatic dissolved organic matter, such as in specific UV absorbance (SUVA) measurements [12,13], but both air bubbles and inorganic particles absorb only weakly at 254 nm, making it unsuitable as a basis for bubble discrimination.

As an alternative approach, this paper proposes a multi-wavelength scattering–absorption hybrid method that exploits the wavelength-dependent absorption characteristics of water itself as the medium. Because water exhibits distinct absorption bands in the near-infrared region originating from overtones of the O–H vibrational mode [14,15], its absorption behavior changes dramatically depending on whether the optical path is occupied by water or by air (bubbles). This difference provides a potential basis for bubble–particle discrimination in water-based monitoring systems.

The main contributions of this paper are as follows. First, a novel spectroscopic bubble–particle discrimination principle is proposed by combining the ISO 7027-compatible 850 nm band with a water-absorption band at 1450 nm; this principle is a universal structure applicable across all water industry sectors. Second, the sample/reference ratiometric dual-detector architecture, previously demonstrated in NDIR gas sensors, is extended to water quality measurement to provide compensation against source drift and optical-window fouling [16,17]. Third, the feasibility of the proposed method is quantitatively evaluated through simulations based on an extended Beer–Lambert formulation and literature-based optical constants.

2. SENSOR SYSTEM DESIGN

2.1 Wavelength selection and physical rationale

Fig. 1 shows the absorption spectrum of pure water over the wavelength range of 400–1900 nm, together with the three wavelengths selected in this study. According to the experimental data reported by *Pegau et al.* and *Segelstein et al.*, the water absorption coefficient, $a(\lambda)$, varies by more than four orders of magnitude across this range and exhibits distinct absorption bands associated with overtones and combination bands of the O–H vibrational modes [14,15]. Table 2 summarizes the water absorption coefficient at each selected wavelength and its corresponding optical role in the proposed sensor system.

Notably, the absorption coefficient of water at 1450 nm is approximately 700 times greater than that at 850 nm. For an optical path length of 10 mm, the transmittance of pure water at 1450 nm is about 5.5×10^{-13} , indicating that the incident

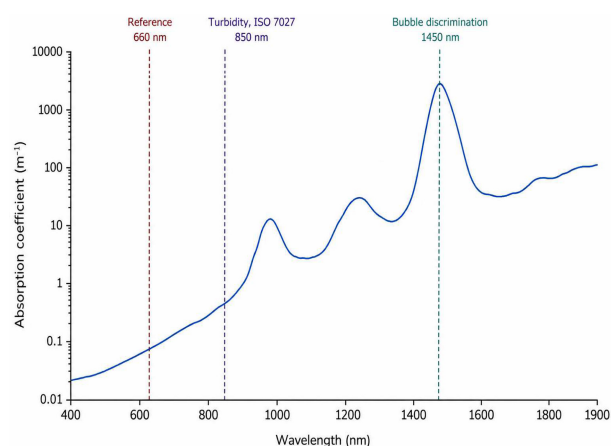


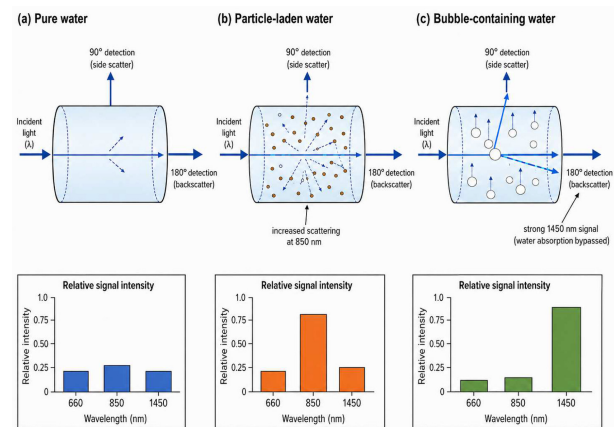
Fig. 1. NIR absorption spectrum of pure water and the three wavelengths (660 nm, 850 nm, 1450 nm) selected in this study.

Table 2. Water absorption coefficient and optical role of each selected wavelength.

Wave length (nm)	Absorption coefficient a_w (m^{-1})	Optical role	Basis
660	≈ 0.4	Reference channel	Low-absorption window
850	≈ 4.3	Primary turbidity measurement	ISO 7027 [4]
1450	$\approx 2,900$	Bubble discrimination	O–H overtone peak [14,15]

light is almost completely absorbed; absorption by air over the same path length is negligible. This substantial difference in absorption forms the physical basis for the wavelength-selective sensitivity to changes in the medium composition along the optical path. Because this principle relies on the intrinsic absorption characteristics of water, it may be broadly applicable to water-based monitoring systems, including those involving ultrapure water, drinking water, wastewater, and process water.

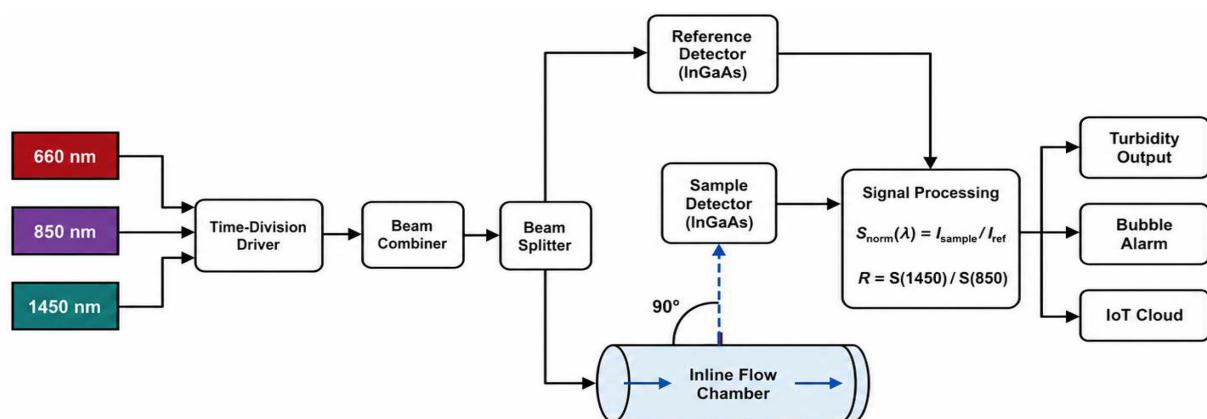
Fig. 2 illustrates this principle using three representative scenarios. In Panel (a), representing pure water, the optical path is completely filled with water, so light at 1450 nm is strongly absorbed and the signal reaching the detector is very low. In Panel (b), representing particle-laden water, the optical path is still occupied by water, so the 1450 nm absorption is maintained, whereas the scattering signal at 850 nm increases due to the presence of suspended particles. In Panel (c), representing bubble-containing water, part of the water in the optical path is replaced by air, thereby reducing absorption at 1450 nm and substantially increasing the corresponding detector signal. Thus, an increase in the 1450 nm signal relative to the water-filled condition can serve as an optical indicator of the presence of bubbles.

**Fig. 2.** Conceptual illustration of absorption and scattering behavior along the optical path for three scenarios: (a) pure water, (b) particle-laden water, and (c) bubble-containing water.

2.2 Optical system and signal processing architecture

Fig. 3 presents an integrated view of the optical system layout and the signal processing flow of the proposed sensor. Three LED sources (850 nm, 1450 nm, and 660 nm) are driven sequentially by time-division multiplexing (TDM) and combined into a single optical path through a beam combiner. The combined beam is then divided by a beam splitter into two paths: one is guided directly to the reference detector without passing through the sample, while the other enters an in-line flow chamber.

Inside the sample chamber, light scattered by suspended particles or bubbles is collected by the sample detector positioned at 90° with respect to the incident beam. To ensure sufficient sensitivity at 1450 nm, extended-range InGaAs photodiodes covering the 900–1700 nm spectral range are employed. Sapphire or quartz optical windows are used to provide sufficient transmission at 1450 nm. The in-line flow

**Fig. 3.** Integrated optical layout and signal-flow block diagram of the proposed three-wavelength time-division LED system with a sample/reference ratiometric dual-detector architecture.

chamber is designed with a standardized flange interface to facilitate integration into various water-industry systems, including drinking- and drainage-water pipelines, aeration tank outlets, bottling lines, ultrapure-water piping, and pipes located upstream of membrane modules.

To compensate in real time for measurement errors arising from source-intensity fluctuations, optical-window fouling, and temperature drift, parallel sample and reference channels are configured for each wavelength. This sample/reference configuration is based on an established architecture commonly employed in NDIR gas sensors and spectrophotometers [16,17]. The measured signal is normalized as

$$S_{\text{norm}}(\lambda) = \frac{I_{\text{sample}}(\lambda)}{I_{\text{reference}}(\lambda)} \quad (1)$$

This configuration is designed to compensate for three major sources of measurement error. First, variations in LED output caused by temperature and aging are common to both channels and thus cancel in the ratio. Second, attenuation caused by fouling of the sample-side optical window is partially cancelled, thereby extending maintenance intervals; this is particularly beneficial in wastewater treatment facilities and raw-water intake sections, where optical-window fouling can be significant. Third, because both detectors share the same thermal environment and drift together, temperature-dependent drift can also be reduced.

2.3 Definition of the discrimination index

By extending Beer–Lambert law to account for scattering, the intensity of the signal reaching the 90°-scattering detector after propagation through an optical path of length L can be expressed as

$$S(\lambda) = I_0(\lambda) \cdot [1 - e^{-(b_p + b_b)L}] \cdot e^{-\alpha_w(\lambda)f_w L} \quad (2)$$

where α_w is the absorption coefficient of water, b_p is the scattering attenuation coefficient associated with particles, b_b is the scattering attenuation coefficient associated with bubbles, and f_w is the volume fraction of water in the optical path ($f_w < 1$ when bubbles are present).

Using the normalized signals of the three wavelengths, the bubble–particle discrimination index R is defined as

$$R = \frac{S_{\text{norm}}(1450)}{S_{\text{norm}}(850)} \quad (3)$$

When bubbles are present, f_w becomes less than unity, thereby reducing the water-absorption contribution at 1450 nm in Eq. (2) decreases sharply; $S(1450)$ therefore rises relatively and R increases. When only particles are present, f_w remains

approximately unity and both wavelengths undergo similar increases in the scattering component, so R remains close to its baseline value. This wavelength ratio is robust against variations in source intensity, optical path length, and absolute turbidity level of the medium, which supports the expectation of consistent discrimination performance across the wide range background turbidity levels encountered in different applications (for example, ultrapure water < 0.1 NTU, raw water < 100 NTU, and sewage < 1000 NTU).

3. OPTICAL MODELING METHOD

3.1 Simulation setup

Based on Eqs. (2) and (3), wavelength-resolved signal responses were calculated for the three simulated scenarios. Table 3 summarizes the simulation parameters and conditions. A turbidity range of 1–500 NTU was considered to represent a broad range of water quality conditions relevant to water-industry applications.

The wavelength-dependent water absorption coefficients were obtained by interpolation of the experimental data reported by Pegau *et al.* [14]. The particle scattering coefficient was derived from a Mie-theory approximation [18] over a log-normal particle-size distribution (0.5–10 μm). An optical path length of $L = 10$ mm and a scattering angle of 90° were assumed.

3.2 Data processing

For each scenario, $N = 80$ repeated calculations were performed, with simulated measurement noise corresponding to a standard deviation of 5% added to each calculated signal to approximate hardware-related variability. The discrimination index R was normalized by the median value obtained for the pure-water scenario, so that $R_0 = 1$. The threshold of $R_{\text{th}} = 2.0$ was selected based on the following rationale. First, as

Table 3. Optical Modeling scenarios and conditions.

Scenario	Water volume fraction f_w	Particle concentration C_p (NTU)	Void fraction (%)	Representative applications
A: Pure water	1.00	0	0	Ultrapure water, purified water
B: Particle-laden water	1.00	1-500	0	Raw water, wastewater influent
C: Bubble-containing water	0.70-0.95	0	5-30	Aeration tanks, bottling lines, upstream of membranes

Table 4. Sensitivity of classification accuracy to the choice of R_{th} .

R_{th}	Pure water (%)	Particle-laden (%)	Bubble-containing (%)	Overall (%)
1.50	100.0	96.3	100.0	98.8
1.75	100.0	97.5	100.0	99.2
2.00	100.0	98.8	100.0	99.6
2.25	100.0	100.0	100.0	100.0
2.50	100.0	100.0	98.8	99.6
3.00	100.0	100.0	96.3	98.8

described in Section 2.1, the substantial difference in water absorption between 1450 and 850 nm causes R to increase as the water fraction, f_w , decreases in the presence of bubbles. Accordingly, $R_{th} = 2.0$ was selected as an intermediate threshold above the particle-response baseline ($R \approx 1$) and below the expected bubble-response range. Second, a simple sensitivity analysis was performed by varying R_{th} between 1.5 and 3.0 in steps of 0.25, and the resulting classification accuracies are summarized in Table 4. Across this range, the overall accuracy varied by less than 2 percentage points, indicating that the classification performance is not overly sensitive to the exact choice of R_{th} , and that $R_{th} = 2.0$ provides a balanced operating point between false-positive and false-negative rates under the assumed 5% noise level. In field validation, R_{th} is expected to be fine-tuned according to the background absorption level of the specific water matrix.

4. RESULTS AND DISCUSSION

4.1 Wavelength-resolved response for each scenario

Fig. 4 shows the wavelength-resolved normalized signals for the three simulated scenarios. In Panel (a), representing pure water, all three wavelengths exhibit low baseline signals, with the signal at 1450 nm being the lowest because of the strong absorption by water. In Panel (b), representing particle-laden water, the 850 nm signal increases with increasing turbidity, whereas the 1450 nm signal also increases due to particle scattering but remains lower than the 850 nm signal because of the strong water absorption at this wavelength. In Panel (c), representing bubble-containing water, the decrease in f_w with increasing void fraction reduces water absorption at 1450 nm, resulting in a pronounced increase in the corresponding signal and a wavelength-response pattern distinct from that observed for particle-laden water.

The observed wavelength-dependent responses are consistent with the physical principle described in Section 2.1 (Fig. 2). Although Scenarios B and C are difficult to distinguish based on any single-wavelength signal alone, the

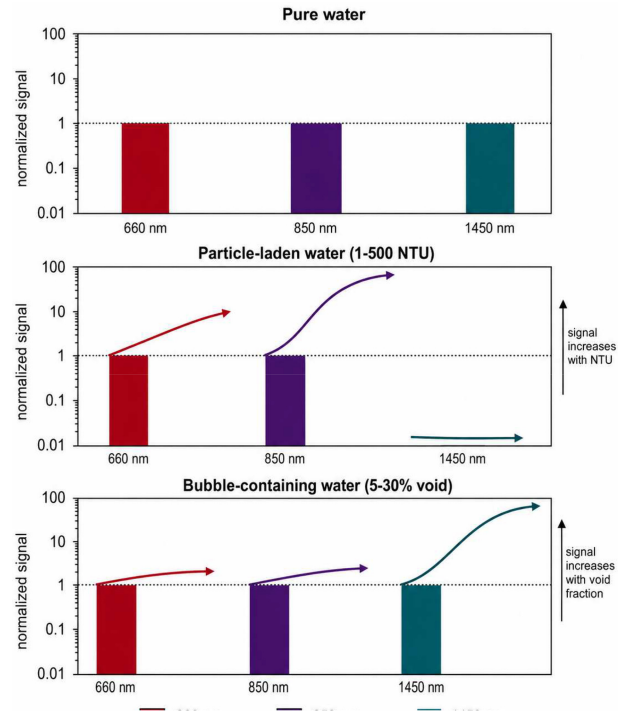


Fig. 4. Simulated wavelength-resolved normalized scattering signals for the three scenarios (pure water, particle-laden water 1–500 NTU, and bubble-containing water 5–30% void fraction).

relative signal ratio between wavelengths provides a basis for discriminating between the two scenarios.

4.2 Distribution of the discrimination index R and classification performance

Fig. 5 shows the distribution of the discrimination index, R , for the three simulated scenarios. Pure water (Scenario A) and particle-laden water (Scenario B) are concentrated near $R \approx 1$, whereas bubble-containing water (Scenario C) is distinctly separated in the range $R = 5$ –50. Table 5 summarized the classification performance obtained using a threshold $R_{th} = 2.0$.

The 1.2% misclassification rate observed for Scenario B occurred primarily at high turbidity levels near 500 NTU, where the combination of strong particle scattering and with the assumed 5% measurement noise shifted some R values toward the classification threshold. It should be emphasized that the accuracy values reported here are obtained from simulations using literature-based optical constants and an extended Beer-Lambert model, and therefore represent a conceptual, simulation-based validation rather than a measured performance of an actual sensor. Most water industry applications operate at much lower turbidity than the boundary case (for example, treated water in drinking-water plants < 1 NTU, bottled water < 0.5 NTU, and ultrapure water < 0.1

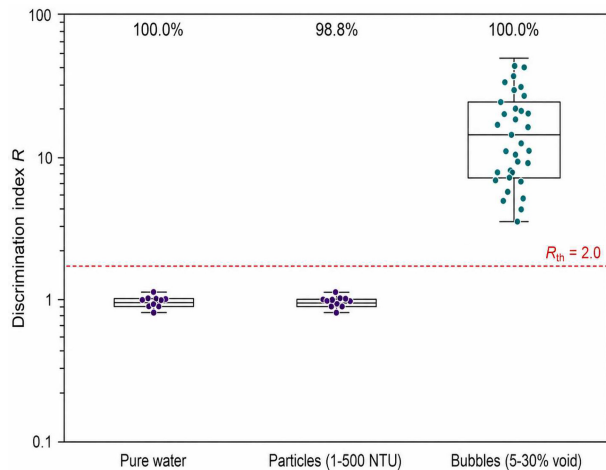


Fig. 5. Distribution of the discrimination index $R = S(1450) / S(850)$ for each scenario and the corresponding classification accuracies at the threshold $R_{th} = 2.0$.

Table 5. Simulated classification accuracy at the threshold $R_{th} = 2.0$.

Scenario	Classification criterion	Accuracy (%)
A: Pure water	$R < 2.0$	100.0
B: Particle-laden water	$R < 2.0$	98.8
C: Bubble-containing water	$R > 2.0$	100.0

NTU), so such boundary cases are unlikely to occur in real operation; however, this expectation itself remains to be verified experimentally.

4.3 Discussion and limitations

These simulation results support the conceptual feasibility of distinguish particles from bubbles by incorporating the water-absorption response at 1450 nm into the discrimination index, R , whereas the 850 nm signal alone does not provide sufficient discrimination between the two scenarios. In particular, the fact that R maintains a constant baseline value independent of the absolute turbidity level supports the universality argument, that is, that a single discrimination logic can be applied consistently across the wide range of background turbidities encountered in different water industry applications, from ultrapure water to sewage. However, these findings are based on proof-of-concept simulations using simplified optical models and should not be interpreted as validation of universal applicability or actual sensor performance. Experimental verification using a physical prototype and representative water matrices is therefore required.

Nevertheless, the present modeling has the following limitations. First, and most importantly with respect to the

discrimination principle, particles and bubbles were considered as independent scenarios rather than as coexisting scatterers in a single optical path. In real water-industry applications, particles and bubbles may coexist, particularly in aeration tanks, coagulation basins, and bottling lines. Under such conditions, their combined effects on scattering and water absorption may alter the discrimination index, R , relative to the independently simulated scenarios. The present study therefore characterizes only the endpoints of this response space, and the transition behavior under coexistence conditions must be evaluated in dedicated follow-up experiments before the method can be regarded as validated for practical deployment. Second, pure water was assumed as the background medium, but in real applications trace organics, minerals, and color-forming constituents can be present, and their background absorption may affect the discrimination index R and, in turn, the optimal threshold R_{th} . The expected effects can be summarized as follows. (i) Colored dissolved organic matter, such as humic and fulvic acids in raw or wastewater, exhibits residual absorption tailing into the visible and near-visible NIR, so background absorption at 660 nm and, to a lesser extent, 850 nm may be increased. This tends to reduce the numerator-relative baseline of R and could shift the pure-water and particle-laden distributions slightly downward, effectively increasing the safety margin against the bubble class. (ii) At very high concentrations of organic matter, weak C-H overtone absorption in bands adjacent to 1450 nm may raise the background of $S(1450)$ and thereby elevate the baseline R , which could reduce the effective margin to R_{th} . (iii) Dissolved minerals such as Ca^{2+} , Mg^{2+} , and Fe species typically show negligible NIR absorption at the selected wavelengths and are not expected to have a first-order effect on R , although Fe-related color may contribute weakly to (i). For these reasons, R_{th} should be treated as a matrix-dependent parameter that is calibrated in situ for each application (for example, a higher R_{th} for organic-rich matrices such as wastewater, and R_{th} close to the present value of 2.0 for clean process water and ultrapure water). Determination of matrix-specific R_{th} values will be one of the primary tasks in the follow-up field validation. Third, the water absorption coefficient at 1450 nm depends on temperature at approximately $0.5\%/^{\circ}\text{C}$ [14], and a temperature-compensation algorithm will therefore be required during field validation. Fourth, hardware-related factors including the spectral responsivity and dark current of the InGaAs detector and the spectral bandwidth of the LEDs, were not fully incorporated into the present model. Finally, changes in the Mie-scattering characteristics of bubbles across the size distribution (from several μm to several mm) may influence the choice of R_{th} , and application-specific quantification through field data will be required.

5. CONCLUSION

In this study, a multi-wavelength scattering-absorption hybrid sensor was conceptually designed and evaluated for bubble-particle discrimination in optical water quality monitoring by exploiting the wavelength-dependent near-infrared absorption characteristics of water. It is emphasized at the outset that the validation reported here is entirely simulation-based, using literature optical constants and an extended Beer-Lambert model under scenarios in which particles and bubbles are treated independently; the reported classification accuracies therefore represent conceptual, proof-of-concept results rather than measured sensor performance. The main findings are summarized as follows.

(1) Physical rationale for wavelength selection: Based on literature evidence, a three-wavelength set was derived that combines 850 nm for turbidity measurement in compliance with ISO 7027, 1450 nm — the strong absorption band originating from the overtone of the O–H vibrational mode of water — for bubble discrimination, and 660 nm as a low-absorption reference for source compensation. The nearly 700-fold difference in the absorption coefficient between 850 nm and 1450 nm provides the physical basis for optically distinguishing bubbles from particles, and this principle constitutes a universal structure applicable to any application in which water is the medium.

(2) Academic justification of the optical architecture: A ratiometric dual-detector architecture, in which sample and reference channels are separated, was adopted to secure real-time compensation for source-intensity fluctuations, optical-window fouling, and temperature drift. This represents an extension of a well-established architecture from NDIR gas sensors to water quality measurement, and it physically guarantees long-term stability and reproducibility from wastewater environments with severe optical-window fouling to drinking-water and industrial-water environments that demand long-term uninterrupted operation.

(3) Conceptual simulation-based validation of the discrimination principle: Simulations based on the extended Beer-Lambert formulation and literature optical constants confirmed that the discrimination index $R = S(1450) / S(850)$ can optically separate the bubble scenario ($R > 5$) from the pure-water and particle-laden scenarios ($R \approx 1$). At a physically motivated threshold $R_{th} = 2.0$, whose choice was further supported by sensitivity analysis over $1.5 \leq R_{th} \leq 3.0$, the three independently simulated three scenarios were classified with accuracies of 98% or higher. These accuracy values are simulation-based indicators of the concept's feasibility rather than a claim of achieved sensor performance, and they were obtained under separately controlled conditions rather than

under particle-bubble coexistence.

(4) Directions for future work. Prototype fabrication and field validation across diverse water industry applications — including drinking-water treatment plants, wastewater treatment facilities, food and beverage process water, and industrial water — are required. The most critical among these is experimental validation under particle-bubble coexistence conditions, which was not covered by the present simulation scope and which is essential for establishing the robustness and practical applicability of the proposed discrimination method. Application-specific effects of background constituents (organics, color, minerals) on the discrimination index and matrix-dependent calibration of R_{th} , real-time compensation of the temperature dependence of the 1450 nm absorption, and quantitative determination of the threshold as a function of bubble-size distribution are additional subjects for future experimental research. Furthermore, integration with AI-based time-series prediction models is planned as a route toward an intelligent water-management platform at the level of predictive maintenance, which is also aligned with the national policy goal of smart water management.

CRedit Authorship Contribution Statement

Jihye Choi: Conceptualization, Methodology, Investigation, Writing – original draft. **Ah Rim Jeong:** Formal analysis, Data curation, Visualization, Writing – original draft. **Dongwoo Lee:** Investigation, Methodology, Software. **Jae-woong Bang:** Supervision, Project administration, Funding acquisition, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This research was supported by the 2026 Water Enterprise Commercialization Support Program (Challenge, Smart Field) of the Korea Environment Corporation.

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