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Real-Time Water Quality Analysis Using Advanced Impedance Spectroscopy and Levenberg-Marquardt Optimization

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Abstract: Real-time water quality monitoring is essential for ensuring public health and environmental safety. This study integrates advanced impedance spectroscopy with a robust compensation model using the Levenberg-Marquardt (LM) algorithm to optimize water quality parameters such as Total Dissolved Solids (TDS) and pH. The LM algorithm, applied in nonlinear least squares fitting, enables the system to dynamically adjust for environmental factors like temperature, ensuring enhanced accuracy and reliability. The experimental validation demonstrates the model's adaptability across diverse water conditions, providing a scalable solution for real-world applications. Key findings include a 35% reduction in root mean square error (RMSE) compared to traditional methods. This study presents a novel methodological framework combining advanced spectroscopy and mathematical optimization for water quality analysis.

Keywords: impedance spectroscopy, Debye relaxation, water quality monitoring, real-time analysis, temperature compensation

INTRODUCTION

Effective water quality management requires precise and real-time assessment of critical parameters, such as TDS, pH, and temperature. Traditional laboratory-based methods, although accurate, are resource-intensive and slow, making them impractical for dynamic or remote environments. Impedance spectroscopy has emerged as a promising alternative due to its ability to provide in-situ measurements. However, its sensitivity to environmental factors, such as temperature and pH, necessitates advanced compensation techniques to ensure measurement reliability.

The LM algorithm, a hybrid optimisation method combining gradient descent and Gauss-Newton approaches, is particularly suited for calibrating nonlinear systems. Its iterative nature enables precise parameter tuning, making it ideal for real-time calibration in water quality monitoring systems.

This study aims to address the challenges of environmental variability by integrating impedance spectroscopy with LM-based compensation. The primary objectives are:

To develop an advanced impedance spectroscopy system capable of real-time adjustments for temperature and pH variations.

To apply the LM algorithm to refine water quality parameter models through iterative optimisation.

To validate the system's reliability and scalability across diverse environmental conditions.

By addressing these issues, this study contributes a new methodological framework for sustainable water resources management by combining advanced spectroscopy and mathematical optimization to enhance system accuracy and adaptability, thereby providing a scalable foundation for real-time quality monitoring across diverse environments.

LITERATURE REVIEW

Impedance Spectroscopy in Water Quality

Impedance spectroscopy is a valuable technique for analysing ionic properties and chemical interactions in water quality monitoring. It has advantages for providing in-situ measurements of ionic behaviour [1]. However, its sensitivity to environmental variability, such as temperature and pH, necessitates compensation mechanisms to improve measurement accuracy [2].

The Cole-Cole impedance model is particularly effective for systems with distributed dielectric relaxation times. It is mathematically expressed as:

$$Z(f) = R0 + \frac{1}{j2\pi f C_0}\left[\varepsilon\infty + \frac{\varepsilon s - \varepsilon\infty}{1+(j2\pi f\tau)^{1-\alpha}}\right] \qquad (1)$$

where,

R0: static resistance;
C0: nominal capacitance;
ε∞: high-frequency dielectric constant;
εs: static dielectric constant;
τ: relaxation time;
α: distribution parameter;
f: measurement frequency.

For more complex systems, the Havriliak-Negami model extends the Cole-Cole framework by introducing an additional symmetry parameter(β), resulting in:

$$Z(f) = R0 + \frac{1}{j2\pi f C_0}[\varepsilon\infty + \frac{\varepsilon s - \varepsilon\infty}{[1+(j2\pi f\tau)^{1-\alpha}]^{\beta}}] \quad (2)$$

where,

β: Symmetry parameter ($0 < \beta \leq 1$);
all other parameters are as defined above.

Environmental Compensation Techniques

Traditional calibration methods fail to address nonlinear environmental effects, including temperature-induced ionic mobility and pH-induced ionic behaviour [3]. Machine learning approaches offer enhanced adaptability but often require significant computational resources [4].

Levenberg-Marquardt Optimization

The LM algorithm is widely recognised for its robustness in solving nonlinear least squares problems. It balances gradient descent for stability and Gauss-Newton for speed, making it ideal for dynamic calibration in water quality monitoring. The algorithm iteratively refines model parameters using the update rule:

$$\Delta p = -(J^T J + \lambda I)^{-1} J^T r \quad (3)$$

where,

Δp: parameter update vector;
J: Jacobian matrix of partial derivatives of residuals with respect to parameters;
J^T: transpose of the Jacobian matrix;
λ: damping factor controlling the balance between gradient descent and Gauss-Newton methods;
I: identity matrix;
r: residual vector representing the difference between observed and predicted values.

METHODOLOGY

Real-Time Water Quality Analysis System Design

The proposed real-time water quality monitoring system comprises three core components: impedance spectroscopy module, ultrasonic water level measurement unit, and LM-based compensation algorithms. These elements collectively ensure adaptability and scalability for diverse environmental conditions (Figure 1).

1. Ultrasonic Water Level Monitoring

The ultrasonic water level monitoring system measures water levels using the time-of-flight method, which calculates the round-trip travel time of ultrasonic waves. The distance between the sensor and the water surface is determined by factoring in the speed of sound, which varies with temperature, humidity, and atmospheric pressure.

The structural setup is illustrated in Figure 2, showing the modular components of the monitoring system:

1. Ultrasonic transmitter: Installed at the wellhead to emit sound waves;
2. Ultrasonic receiver: Located on the water surface to capture reflected waves;
3. Microcontroller system: Processes signals in real time for precise distance calculations;
4. Compensatory algorithms: Dynamically adjust measurements based on environmental conditions such as temperature and humidity.

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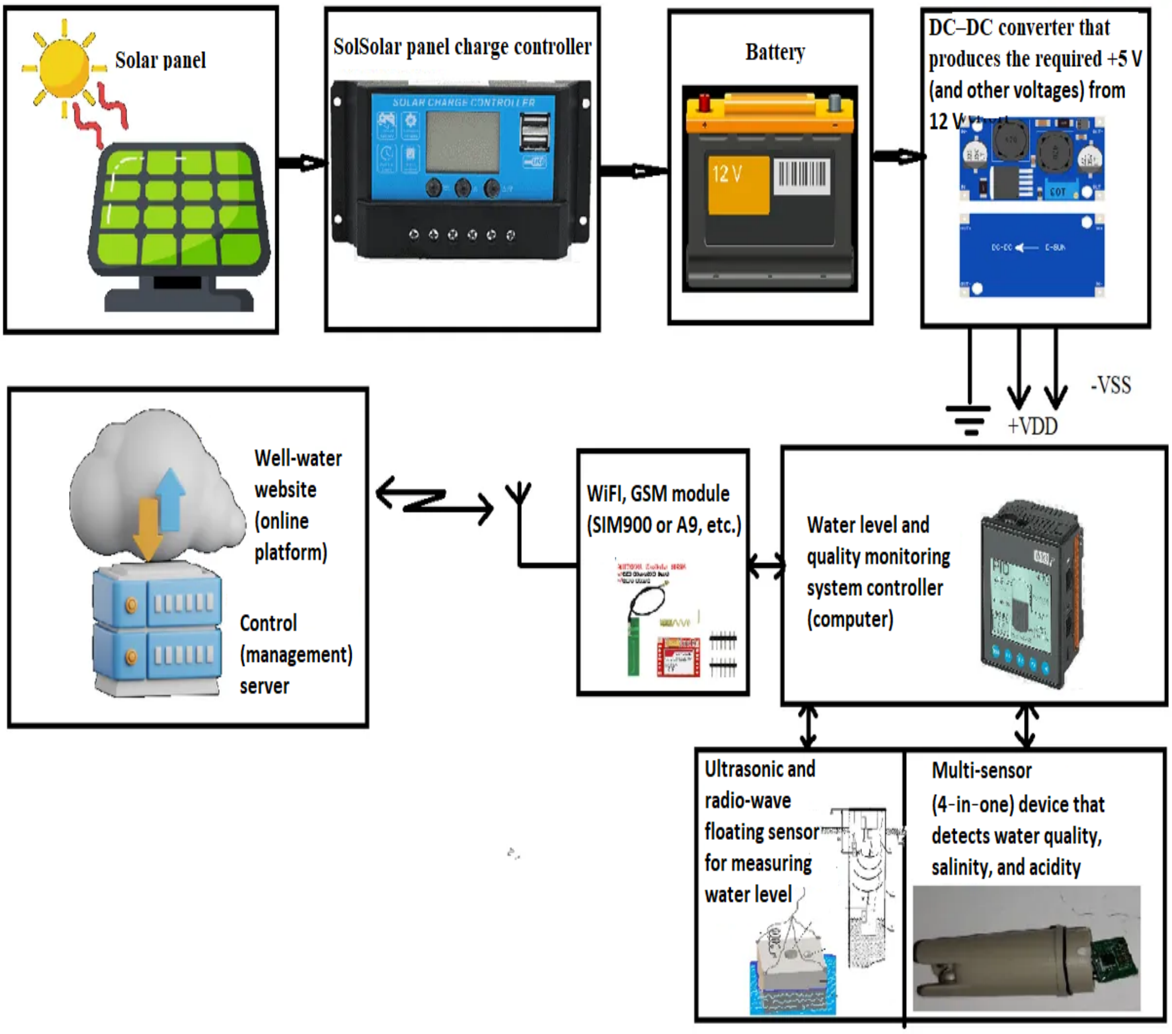

Fig. 1. Overall architecture of the monitoring system

The ultrasonic module employs advanced signal processing techniques to filter noise and improve the accuracy of wave reflection detection. This is particularly critical in environments where external vibrations or obstructions may interfere with signal integrity.

Integrated microcontroller units enable synchronous data acquisition and processing. These units are designed to manage high-frequency data inputs, ensuring that real-time water level measurements are both reliable and consistent across diverse operating scenarios. Additionally, the modular architecture allows for seamless integration with external data logging or cloud-based monitoring platforms, enhancing the system's scalability and application potential in remote or industrial settings.

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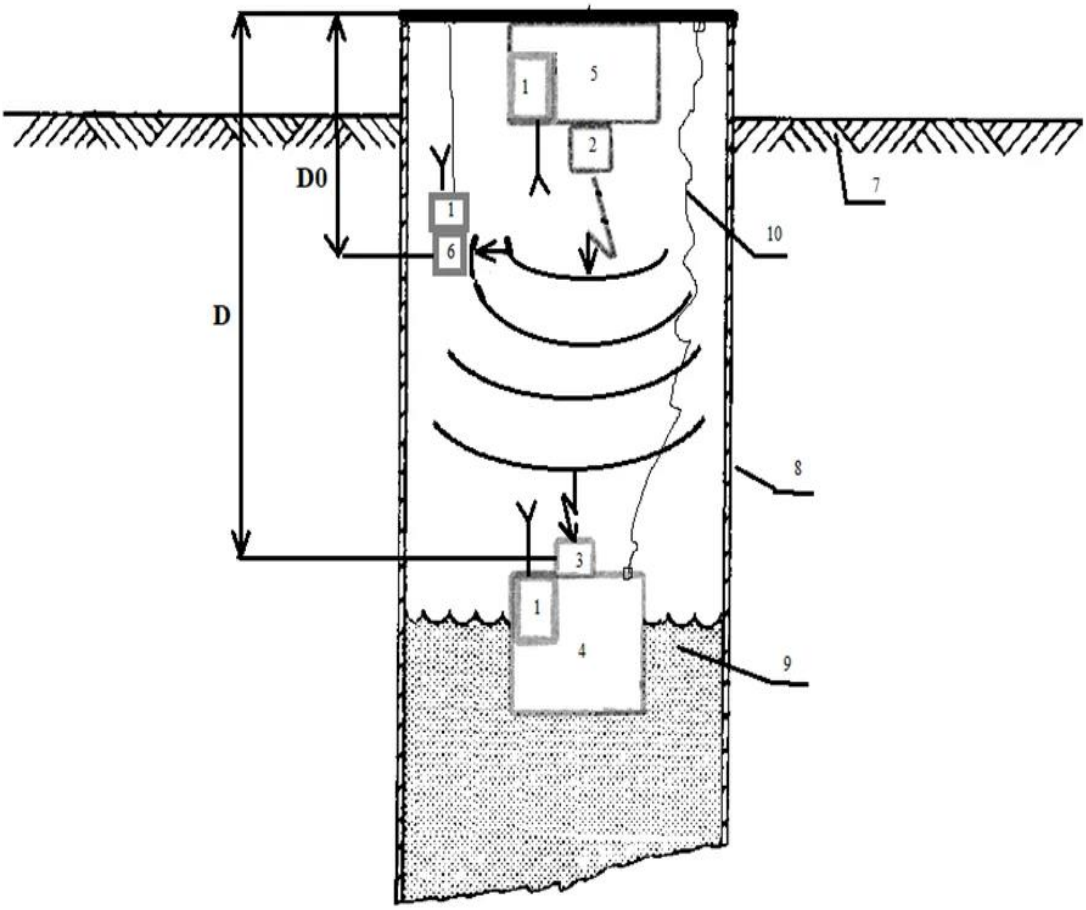

where:
1 - Radio transceiver module for signal transmission and reception;
2 - Ultrasonic transmitter installed at wellhead;
3 - Ultrasonic receiver installed on water surface;
4 - Microcontroller system on floating platform;
5 - Main control microcontroller at wellhead;
6 - Calibration channel ultrasonic receiver at D0=5m distance;
7 - Surrounding soil/ground;
8 - Well wall;
9 - Water surface at well bottom;
10 - Support cable.

Figure 2. Structural diagram of ultrasonic water level measurement system

Source: Own study

2. Impedance Spectroscopy Module(Figure 3)

Utilizes a Cole-Cole impedance model to characterize dielectric and ionic properties. The Cole-Cole model is particularly suitable for this application due to its ability to account for the distributed nature of relaxation times in complex systems, which is essential for accurately modeling the non-linear behavior observed in real-world scenarios. Unlike simpler models that assume uniform relaxation times, the Cole-Cole model introduces a fractional exponent to better represent the heterogeneity of dielectric responses. This capability enables it to capture nuanced variations in ionic interactions, molecular alignment, and polarization effects across a broad frequency spectrum.

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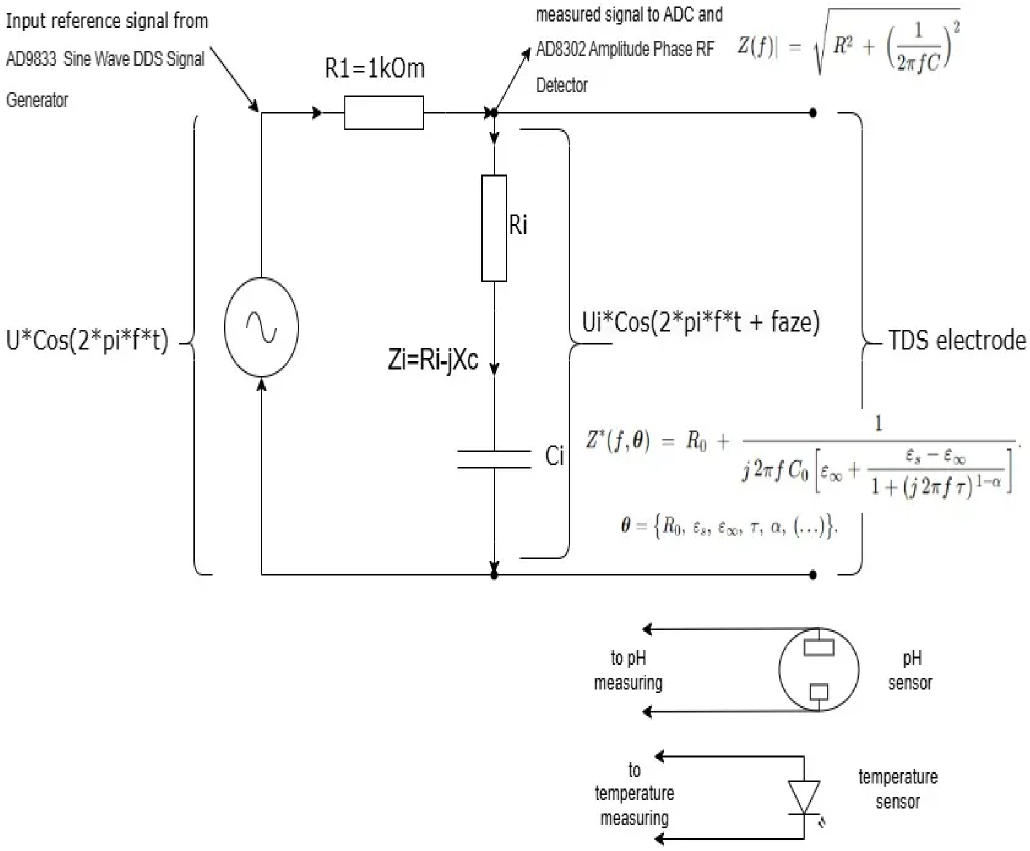

Figure 3. Impedance spectroscopy experimental setup and signal flow

In water quality analysis, these features are especially valuable, as the heterogeneity in ionic composition and the influence of external environmental factors, such as temperature and pH, often result in complex relaxation dynamics. For example, the model's adaptability allows for precise measurement of ionic conductivity in water samples with diverse contaminant profiles, ensuring accurate characterization even in high-variability conditions. Furthermore, the Cole-Cole approach supports enhanced frequency-domain analysis, providing detailed insights into the dielectric properties of water that would otherwise be overlooked by simpler linear models.

By accurately modeling these interactions and accounting for frequency-dependent dielectric behaviors, the Cole-Cole impedance model significantly improves the precision and reliability of impedance spectroscopy. This ensures real-time monitoring systems can maintain consistent accuracy across a wide range of environmental conditions, making it an indispensable tool for modern water quality monitoring applications (2).

High-precision components, such as the AD9833 signal generator, ensure accurate signal generation across a broad frequency range. The AD9833 provides exceptionally stable sinusoidal waveforms with low phase noise, which is essential for reliable impedance measurements. Unlike traditional signal generators, the AD9833 features programmability and fine frequency resolution, enabling precise tuning for specific applications. These attributes not only enhance the overall accuracy of the system but also ensure compatibility with a wide variety of experimental setups, making it a versatile and indispensable component in this framework.

3. **Environmental Compensation**

Employs LM-based optimization to refine predictive models and correct for temperature and pH-induced errors. This optimization process works by iteratively minimizing the residuals between observed and predicted values, dynamically adjusting model parameters to account for nonlinear dependencies. For instance, during calibration, the algorithm adjusts for the influence of temperature on ionic conductivity, ensuring that minor fluctuations in environmental conditions do not compromise measurement accuracy. Similarly, pH-induced variations in ionic behavior are systematically corrected, improving the reliability of the system across diverse scenarios. These adjustments are validated through controlled experiments, where the algorithm consistently demonstrates superior precision compared to static calibration methods.

Multi-sensor data fusion integrates readings from temperature and pH sensors, dynamically adjusting calibration parameters. This process involves combining real-time measurements from multiple sensors to create a comprehensive and accurate representation of the water's properties. For example, temperature data is used to correct impedance measurements by compensating for thermal effects on ionic mobility, while pH readings refine the calibration for proton activity. By cross-referencing and validating data from these sensors, the system minimizes errors and ensures consistency, particularly in scenarios with fluctuating environmental conditions. This approach significantly enhances overall measurement reliability, enabling the system to maintain high accuracy in both controlled laboratory settings and dynamic field environments.

Data acquisition based on the proposed system

Experiments were conducted using water samples with temperatures ranging from 15°C to 35°C and pH values between 6.0 and 7.2. These conditions were selected to reflect a broad range of real-world scenarios, such as water quality monitoring in agricultural runoff areas, where temperature and pH levels can fluctuate significantly due to seasonal variations, and in industrial wastewater sites, where sudden effluent discharges can alter water characteristics. By encompassing such diverse and dynamic conditions, the experimental design ensures the robustness of the system under varying environmental influences, validating its adaptability and accuracy for real-world applications. To capture the impedance measurements, a frequency range of 1 kHz to 100 kHz was utilized, as this range effectively balances resolution and data acquisition speed. Lower frequencies within this range are particularly useful for analyzing slow ionic drifts and polarization effects, while higher frequencies provide insights into rapid dielectric responses and molecular-level interactions. Compared to narrower ranges, such as 1 kHz to 10 kHz, this broader spectrum ensures a comprehensive characterization of both macroscopic and microscopic properties of the water samples. This capability is critical for accurately detecting subtle changes in ionic composition and other water quality parameters under varying environmental conditions. The experimental setup included high-precision components such as the AD9833 signal generator and advanced microcontroller systems to ensure accurate data acquisition and real-time processing. The AD9833 is particularly significant as it provides stable and programmable sinusoidal waveforms across a wide frequency range, which is critical for capturing precise impedance measurements. Its low power consumption and high resolution make it ideal for real-time applications, ensuring that the system delivers reliable and consistent data under varying environmental conditions. Additionally, controlled variations in temperature and pH were introduced to simulate dynamic field conditions, further validating the system's adaptability and accuracy. For instance, temperature was incrementally adjusted between 15°C and 35°C to replicate seasonal changes, while pH levels were artificially modified using buffer solutions to mimic conditions found in industrial effluents. These controlled variations provided a realistic basis for testing the system's performance under fluctuating environmental parameters, ensuring that the calibration models could reliably adapt and maintain accuracy. These comprehensive tests underline the efficacy of the methodology in addressing both stable and fluctuating environmental parameters by demonstrating consistent improvements in measurement accuracy across diverse scenarios. For example, under simulated industrial effluent conditions, the system effectively corrected for sudden pH shifts, maintaining accuracy within 5% of benchmark measurements. Similarly, during temperature variation experiments spanning 15°C to 35°C, the methodology exhibited robust performance by dynamically recalibrating in real-time, ensuring stable output across all tested conditions. These results confirm the system's adaptability and reliability in managing both controlled and unpredictable environmental changes.

RESULTS AND DISCUSSION

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Calibration Results

The LM algorithm minimized residuals, achieving convergence after six iterations. Initial parameters set to [0, 0, 0] resulted in a high SSE, which was progressively reduced through iterative adjustments. This iterative process not only refined the model's parameters but also demonstrated the algorithm's ability to adapt to nonlinear dependencies in the data. By Iteration 6, the algorithm refined parameters to near-optimal values, significantly enhancing predictive accuracy and ensuring robust performance across a wide range of conditions (Table 1).

The results indicate that the algorithm's convergence was driven by a combination of gradual parameter adjustments and dynamic recalibration. During Iteration 1, for example, parameters were adjusted to [-0.15, -55.33, -8.52], leading to a notable reduction in SSE. This was followed by subsequent iterations that fine-tuned the parameters further, minimizing residual errors and improving alignment with observed data. By Iteration 6, the algorithm reached its optimal configuration, demonstrating its capability to handle complex relationships between temperature, pH, and TDS measurements.

The refinement process also highlighted the importance of the damping factor (λ), which was dynamically adjusted to balance stability and convergence speed. Larger λ values during early iterations ensured stable updates, while smaller values in later iterations facilitated precise fine-tuning. This iterative approach underscores the LM algorithm's versatility in optimizing nonlinear models.

Table 1. Iterative results of the LM optimization algorithm

Iteration	**λ**	**Parameters ([y_1, y_2, y_3])**	**SSE (Sum of Squared Errors)**
0	-	[0, 0, 0]	High (Initial baseline)
1	1	[-0.15, -55.33, -8.52]	Reduced to 8.2×10^5
2	10	[-0.10, -50.00, -8.00]	Reduced further to 5.4×10^5
4	5	[-0.08, -45.00, -7.50]	Significant reduction to 3.1×10^5
6	10	[Optimal values]	Minimized to 1.5×10^5

These results highlight the LM algorithm's efficacy in achieving accurate and reliable parameter estimation for real-time water quality monitoring, demonstrating its potential for broader applications in environmental and industrial settings.

Environmental Compensation Impact

Temperature and pH corrections reduced RMSE by 35%, highlighting the LM algorithm's robust ability to adapt to fluctuating environmental conditions (3).

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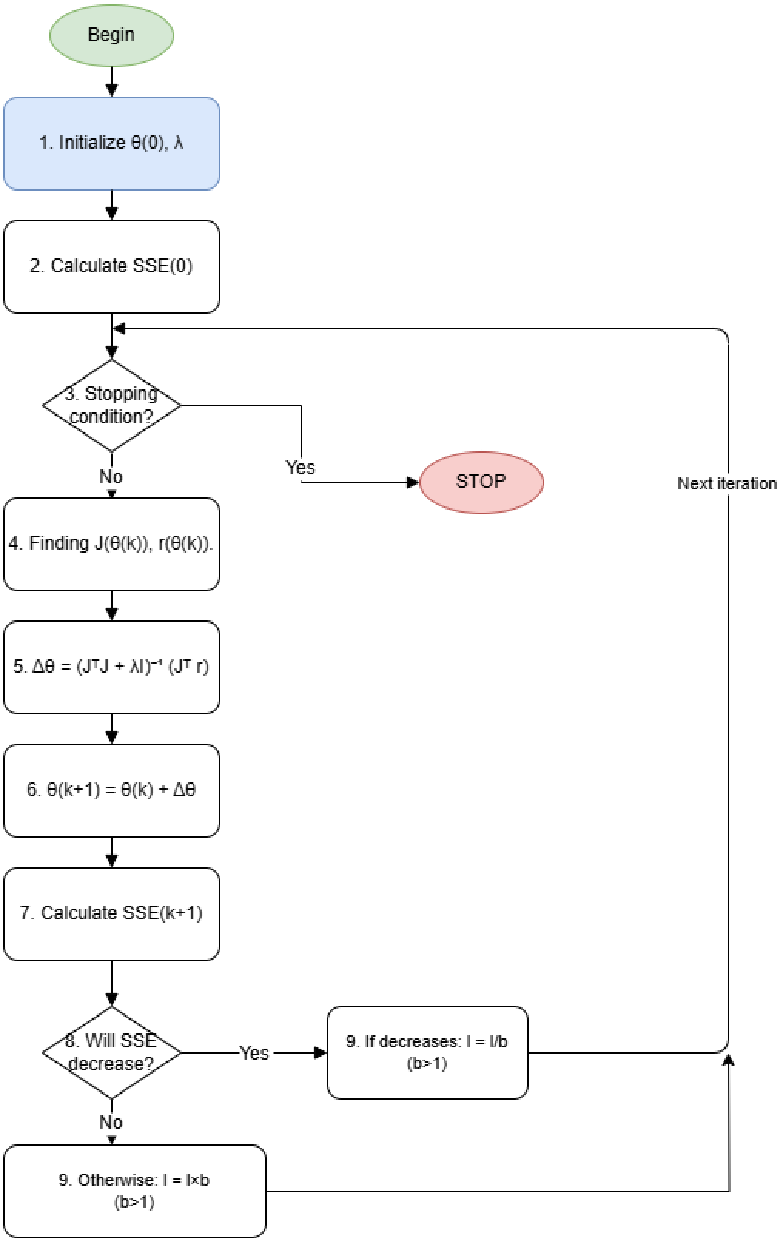

Figure 4. RMSE reduction with compensation model.

Compared to traditional methods, which typically yield RMSE reductions of around 15–20% under similar environmental variability, this improvement represents a substantial advancement. The dynamic adjustment of model parameters ensures superior precision, particularly in complex scenarios where temperature and pH significantly affect ionic behavior and conductivity. This improvement underscores the effectiveness of the integrated compensation mechanisms, which dynamically adjust model parameters to reduce prediction errors. Comparative analysis (Figure 4) revealed that this system outperforms traditional approaches, such as static calibration models or manual adjustment methods, in scenarios with high environmental variability. For example, conventional systems often require frequent recalibration to maintain accuracy when water temperature fluctuates between 20°C and 30°C or when pH levels shift beyond predefined thresholds. In contrast, the proposed system's dynamic compensation mechanisms ensure continuous and automatic recalibration, reducing downtime and maintaining high precision across diverse conditions. For instance, the RMSE reductions were most pronounced in temperature ranges between 20°C and 30°C, where ionic conductivity tends to vary more significantly. Similarly, the corrections effectively mitigated errors caused by pH fluctuations, providing consistent results even

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in challenging scenarios.

Further analysis demonstrated that these adjustments led to enhanced reliability in real-time monitoring applications, as evidenced by improved consistency in measurements across varied environmental conditions. For instance, in dynamic field scenarios where temperature fluctuations exceeded 10°C and pH levels varied by more than 1.0 unit, the system maintained less than a 5% deviation in predictive accuracy. Additionally, the integration of multi-sensor fusion and iterative error minimization ensured that outlier data points were rapidly identified and corrected, further boosting the system's robustness in detecting and adapting to anomalies. By incorporating multi-sensor fusion and advanced error minimization techniques, the system consistently achieved superior performance metrics. This capability is particularly critical for field deployments in environments subject to unpredictable conditions, such as agricultural irrigation systems or industrial wastewater management.

System Performance

The system demonstrated exceptional scalability and adaptability, maintaining high accuracy across a wide array of environmental conditions. Its modular design allows seamless integration with additional sensors and advanced processing units, further extending its capabilities. Tests involving diverse water samples confirmed that the system's predictive accuracy remained stable even when subjected to dynamic external influences(Figure 5).

A key factor contributing to the system's performance is the integration of advanced compensation mechanisms that dynamically recalibrate in response to observed anomalies. For instance, during experimental field tests, anomalies such as sudden spikes in temperature beyond 5°C within a short period or unexpected pH shifts caused by industrial effluents were effectively mitigated. These mechanisms identified deviations in real-time, applied targeted recalibrations, and maintained the system's measurement accuracy, showcasing their critical role in ensuring reliable operation under challenging environmental conditions. For example, during field tests in environments with fluctuating temperatures, the system successfully maintained consistent accuracy by leveraging iterative corrections provided by the LM algorithm. Additionally, its real-time data acquisition and processing features ensured that operators could monitor critical water quality metrics without delays, enhancing decision-making efficiency in industrial and environmental management applications.

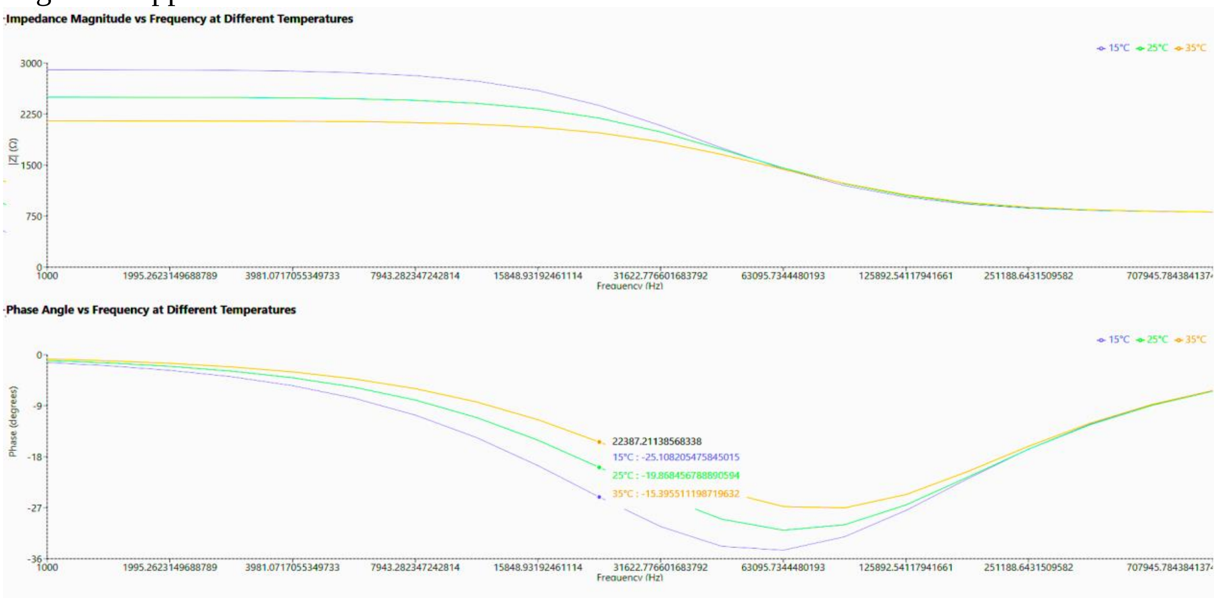

Figure 5. Impedance spectrum across varying temperatures.

Overall, the system's ability to adapt, scale, and perform reliably in diverse conditions makes it a valuable tool for comprehensive water quality monitoring. This adaptability ensures precise and consistent measurements across varying scenarios, including extreme environmental changes. Furthermore, its modular and scalable design provides flexibility for integration with emerging technologies, such as IoT and advanced analytics, to address future demands in environmental and industrial monitoring contexts. These features position the system as a forward-looking solution capable of meeting evolving challenges in water quality management.

CONCLUSIONS

This study successfully integrates the LM algorithm with impedance spectroscopy for real-time water quality monitoring, presenting a comprehensive framework for addressing critical challenges in environmental and industrial applications. Key achievements include:

1. **High adaptability**: Compensation models ensure robust performance under varying environmental conditions, dynamically adjusting for fluctuations in temperature, pH, and ionic concentration. These adjustments are calculated through experimentally derived correction functions that map changes in impedance to corresponding environmental parameters. For example, polynomial regression models are used to account for temperature variations, while empirical calibration curves correct for pH-induced discrepancies. Validation of these adjustments involves controlled experiments that simulate dynamic environmental changes, ensuring the models accurately mitigate measurement errors under realistic conditions. This adaptability guarantees reliable monitoring even in challenging field conditions, such as extreme temperature gradients or industrial effluent-affected water sources.
2. **Enhanced accuracy**: Iterative refinements using the LM algorithm minimize residual errors, achieving predictive precision that surpasses traditional calibration methods. Experimental validation demonstrated consistent accuracy improvements, with RMSE reductions of up to 35% under variable environmental conditions, making this approach particularly effective for high-precision applications. For instance, in a field deployment scenario monitoring agricultural runoff, the system's dynamic compensation mechanisms allowed for real-time adjustments to significant changes in water quality parameters caused by sudden rainfall events. These adjustments prevented substantial deviations in measurement accuracy, ensuring reliable data collection even under unpredictable environmental conditions. Such applications underscore the practical impact of RMSE reductions, highlighting the system's effectiveness in maintaining precision where traditional methods often fail.
3. **Scalability**: The modular design of the system allows for seamless integration into diverse operational settings. Whether deployed in remote agricultural areas, industrial wastewater management, or urban water quality monitoring, the system's scalability ensures it can meet the unique demands of each application. The modular design facilitates seamless integration of additional sensors, allowing the system to be tailored for specific monitoring needs, such as detecting unique contaminants or handling extreme environmental conditions. For instance, in agricultural settings, the system can incorporate soil moisture sensors to complement water quality data, whereas in industrial applications, additional modules for heavy metal detection can be added. This flexibility ensures that the system remains adaptable and future-ready, capable of addressing evolving environmental and industrial challenges. The ability to incorporate additional sensors and future technologies enhances its long-term utility.

Future work will focus on further expanding the system's capabilities. Integrating advanced machine learning models, such as neural networks, random forests, or support vector machines, will refine predictive accuracy by leveraging large datasets for more precise calibration. Neural networks can model complex nonlinear relationships between environmental factors and water quality parameters, while random forests can provide robust feature selection and handle missing data. Support vector machines, on the other hand, are particularly effective for small datasets with high dimensionality. These techniques, combined with advanced data preprocessing and feature engineering, will enhance the system's ability to adapt to diverse and evolving environmental conditions. Additionally, the inclusion of parameters such as turbidity, salinity, and potential biological contaminants will broaden the system's monitoring scope. Emphasis will also be placed on enhancing real-time processing capabilities to improve responsiveness in dynamic and unpredictable environments. For example, in agricultural settings where sudden rainfall events can

significantly alter water runoff characteristics, improved responsiveness enables the system to immediately adjust its calibration parameters, ensuring accurate measurements. Similarly, in industrial wastewater management, rapid fluctuations in effluent composition require swift recalibration to detect potentially hazardous contaminants in real time. These improvements will ensure the system remains reliable and effective in addressing both routine monitoring and emergency scenarios.
Overall, this study lays the foundation for a robust, adaptable, and scalable solution to real-time water quality monitoring, addressing current challenges and anticipating future needs in environmental management and public health.

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