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Novel internet of things-spectroscopy methods for targeted water pollutants in household point-of-use environments

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ABSTRACT

Ensuring water quality remains a paramount concern to prevent adverse health effects on consumers. Water quality monitoring primarily focuses on water utilities and infrastructure, such as treatment plants and reservoirs. More information is needed on the status of water once it enters the consumption phase, particularly at the point-of-use (POU). Therefore, this study aims to provide a scientific understanding of water quality in response to microbial contaminants in Malaysia's household water system using the non-invasive benchtop near-infrared (NIR)-Raman spectroscopy approach. This study also provided the effects of seasonal variations and stagnation periods on the quality of water supply, corresponding to microbial contaminants. Findings show that almost 20% of the water samples contained Legionella and Salmonella species through the Raman spectral identification technique. The distinct signature peaks (ranging from 400 cm-1 to 1,800 cm-1) indicative of specific bacterial species are identified. However, benchtop Raman spectroscopy has application constraints in real-time water quality monitoring. Hence, acknowledging its limitation, this study proposed a new internet of things (IoT)-based micro-spectrometer as an alternative to rapid and sustainable POUs water quality assessment. Leveraging IoT protocols enhances the reliability and efficiency of identifying microbiological threats in water supply.

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1. INTRODUCTION

Ensuring the provision of potable water from surface or ground sources through water distribution systems (WDS) is crucial for meeting state and federal consumption standards. Water operators must prioritize the delivery of reliable and safe water. However, the occurrence of water recontamination during transportation along the distribution system is inevitable and beyond control. Generally, potable water undergoes treatment processes such as sedimentation, filtration, disinfection, and flocculation. However, although efforts have been made to maintain quality of potable water, quite often, but not always, quality of water supply deteriorates substantially along the distribution system [1]. There are several studies investigating the potential contributing factors that causes water quality deterioration during transportation of water from treatment facilities to the level of consumptions. These factors includes the effect of biofilms,

leakages, corrosion, and fecal contaminants significantly contribute to microbial presence in the WDS, posing serious health risks to consumers [2]. Microbial contaminants proliferate downstream, from primary pipelines to smaller diameters within buildings [3]. Isolated areas within domestics plumbing or water system that are not disinfected accordingly, such as dead legs, inducing the growth of microorganism community. While consecutive efforts have been initiated to reduce waterborne outbreaks, achieving sanitation and hygiene targets in household water supply remains a global challenge, with about 88% of diseases attributed to inadequate water safety access [4]. Existence of microorganism activity along water distribution pipeline systems are mainly caused by biofilms formation on internal pipeline surfaces, leading the the substantial growth of microbes and resulted in recontaminantion events [5]. Furthermore, microbes within biofilms can also developed during the installation process of pipe surfaces. Certain pathogenic microorganisms typically exist as free-floating single cells in planktonic form within the WDS. However, upon attaching to pipeline surfaces, they form matrices and establish colonies. These colonies mature within the biofilm matrix, creating a protective shield that makes detecting these microorganisms challenging.

Over time, biofilms disperse into potable water within the distribution system, ultimately reaching consumers. In addition to the factors mentioned, various other circumstances contribute to water deterioration, including aging infrastructure, surface materials, historical breakages, operational parameters, and water age. Research indicates distinguishing difference bacterial species surviving in water ecosystems are extremely time consuming which poses challenges and invasive measures [6]. In addition, several distribution tolpologies and components integrities, such as pipes material, storage facilities, pumping stations, valves and fittings, unintentionally could serve as ideal resources for microbial productivity. Previous studies have observed substantial bacterial growth on pipeline surfaces, including iron and plastic polyvinyl chloride (PVC) pipes [7]. However, iron pipelines appear to be particularly conducive to microbial activity within WDS. Microbes' ability to dominate the corrosion of metals like iron, copper, and aluminum, typically considered corrosion-resistant, poses a genuine threat to potable water quality [8]. On top of that, microbes that survived in low-oxidized pipeline environments can adapt to extreme conditions by altering their bacterial morphologies, including survival growth, species division, and shape-shifting abilities.

With a notable absence of research investigating microbial contaminants, further action particularly in monitoring water quality at point-of-use (POUs) distribution systems is necessary. The central problem related to water deterioration is recontamination occurrences in domestic water systems at household or residential POUs [9]. The evaluation of water quality, emphasizing identification of microbial contaminants in water system, at national level is still at its infancy [10], [11]. Several limitations of recent water quality monitoring techniques, such as the culture-dependent approach and Ribonucleic Acid (RNA)/Deoxyribonucleic Acid (DNA) extraction, are complex, time-consuming, costly, and laborious [12]. Notably, these traditional methods typically analyze data in specified laboratory environments, constraining the ability for real-time monitoring. Hence, they hinder the development of an effective monitoring strategy for detecting contaminants at POU. Therefore, there is a pressing need to understand bacterial community presence patterns in building WDS and stagnant tap water under various pipeline conditions. Most water treatment plants and utilities generally use faecal indicators as a sign of compromised water ecosystems. For instance, the presence of *E. coli* exceeding standard concentration level indicates possible human or animal waste intrusion within distribution systems [13]. Indicator organisms, such as total coliforms, are frequently employed in various water monitoring methods. However, an insignificant correlation exists between these indicators and the type of pathogenic species because the absence of indicators in water does not guarantee the absence of pathogenic microorganisms.

As described above, many monitoring techniques for detecting microbiological contaminants are often cumbersome and complex, requiring further analysis in a laboratory setting after sampling procedures. Recently, water utilities adopted fluorescence and absorbance spectroscopy techniques due to their ability to detect biological quality monitoring through observation of fluorescent dissolved organic matter (DOM) that correlates to the presence of *E. coli* bacteria [14], [15]. A study demonstrates the ability of fluorescence spectroscopy to detect bacterial intrinsic fluorophores based on chemical cell compositions: amino acids, flavins, and nicotinamide nucleotide transhydrogenase, resulting in the identification of *bacillus subtilis*, *staphylococcus aureus*, *Escherichia coli*, and *pseudomonas aeruginosa* [16]. However, DOM in the water system can emit fluorescence, which sometimes interferes with or masks bacterial fluorescence signal due to its high signal intensities, potentially leading to false identification. Such limitations have recently led to increased interest towards spectroscopic techniques for assessment of water quality in ecosystems. To overcome this weakness, infrared (IR), near-infrared (NIR), and Raman spectroscopy techniques provide complementary technologies for precisely detecting microorganisms in water environments. This vibrational spectroscopy is a relatively simple but rapid and precise method, interpreting the "fingerprint regions" that correspond to critical functional groups that provide information associated with untargeted species [17]. The essential advantages of NIR and Raman instrumentation are non-destructive, with little to no sample

preparation, and the ability to distinguish diverse bacterial species without extra processing procedures, typically involving three processes: sample collection, sample scanning, and spectrum analysing [18]. Leveraging spectroscopic approaches enables a more practical technique for rapid bacterial identification in WDS.

Therefore, this study provides understanding of the microbial epidemiology in household water delivery infrastructure, leveraging more effective microbiological monitoring and pathogen detection in complex natural settings. This study was inspired by the need to provide a better, sustainable water quality monitoring effort, ensuring the safety of the water supply. Whenever possible, chemical sampling of the water should coincide with biological sampling so that quality metrices of samples can all be correlated with one another. Hence, this study utilizes the NIR-Raman spectroscopy approach for the identification of microbes in response to pH level and water temperature at household POU locations. Three areas of interest were addressed in this study: i) the microbial communities living in the household water ecosystem, ii) quality factors affecting and influencing these communities, and iii) advances in real-time monitoring technology that is needed to study these communities effectively. Ideally, it is necessary to establish a reliable monitoring strategy that works diligently for the determination of the specific microbes that occupy household or residential POUs and understand species epidemiology in the ecosystem. However, that still represents a significant gap in knowledge.

As highlighted above, available water monitoring techniques need to focus on monitoring the quality of water at the consumption level. The majority of WQM applications are placed on treatment facilities and several water base stations, concentrating on the quality of water resources rather than the water that is delivered to users. Hence, this leads to data scarcity related to events of contamination at residential or household POUs. Consequently, small datasets could not provide a thorough insight into microbial contamination events within the WDS, as the quality of water constantly fluctuates over time. Additionally, no quantitative study and explicit monitoring have been done in Malaysia dedicated to the identification of targeting microbial contaminants within the household WDS [19]. The true diversity of microbes that presence in residential water network systems for once can be studied, particularly at POU locations. The scientific understanding and technological advancement necessary to characterize microbes in household water systems come at a time when the need to make informed decisions about upgrading and optimizing quality water supply at POUs has never been greater. Aiming to fill the research gap, this study offers an alternative solution for the detection of microbial contaminants in domestic water used at household POUs. Thus, the significant contribution of this study is:

- Fist-hand information on household POUs' water quality variables affecting microbial composition within the domestic water pipeline system in response to natural environmental settings and water stagnation periods.
- Non-invasive and reliable microbial identification methods using rapid NIR-Raman spectroscopy based on fingerprint spectral analysis in response to quality parameters.
- Introduction of novel intelligent portable spectrometer device for contaminants detection at POUs regions, capable of real-time evaluation via water quality index (WQI) monitoring.

The article is structured as follows: section 2 described the methodology used in this work, highlighting the approach and technique used for the identification of contaminants. Section 3 provides the details of the results and a discussion, with an evaluation of the types of contaminants detected in the POU regions. Moreover, it also introduces a proposed detection device and appropriate design to monitor water quality at household POUs adequately. Finally, section 4 concludes this study.

2. METHOD

Following the MWA design guidelines for water supply systems, comprehensive guidance on water supply management systems was collaboratively developed by water-related institutional stakeholders from both the public and private sectors [20]. This section described the detail methods used for data sampling, quality parameters examination, microbial identification, and data analysis.

2.1. Data sampling

The sampling sites compose various residential POU tap water sources in student residencies and household buildings at Skudai Regions, Johor, Malaysia, encompassing sampling areas of 1,148 hectares. The primary water supply was obtained from the local water authority, which manages potable water distribution in the region and originates from Gunung Pulai Water Treatment Plant. The sampling occurs during the shifting climate from heavy monsoon season (November 2017 to January 2018) to dry season (mid-February 2017 to April 2018). As for the evaluation of water quality during stagnation periods, the sample was collected during mid-semester breaks with three-week intermittent usage. Areas of tap water

samples with consistent and smooth water flow were considered meticulously to observe any potential microbial present within the distribution system. Taps with intermittent flows were later selected to reflect water quality during stagnation periods, as temporary fluctuations can inhabit clumps of potential microbial contaminants in residential plumbing systems [21]. Water quality evaluation was done only on samples collected at residential standpipes. No analysis was conducted on water entering the distribution system. Following the WHO *Guidelines for Drinking Water Quality*, 288 water samples were collected within six months, considering the sufficient sample size recommended for water distribution networks in residential regions. As for stagnation analysis, 120 water samples were collected within three weeks, with pre-stagnation evaluation in the first week of March 2018 and post-stagnation samples collected three weeks later. The sample was collected in exact monthly locations using 100 mL borosilicate glassware, calculating the mean value of three measurements taken. Prior to collecting water samples, in situ measurements of physical parameter; pH and temperature, were conducted at every sampling location. No storage or preservation steps were required.

2.2. Quality parameters examination

The health status of water was evaluated according to the quality standards provided by the EPA's National Standard for Drinking Water Quality. Although a pH value of 7 is considered ideal for drinking water, the recommended quality level for pH must lie between the range of 6.5-8.5 [22]. Generally, drinking and tap water temperature evolves around 25 °C; however, wherever possible, the temperature should ideally be outside the range of 25–50 °C to hinder the growth of microorganisms [23]. The optimum pH range for the growth and survival of most targeted microorganisms in water environments based on WHO quality standard [24]. Measurements that were not within acceptable range were taken to the laboratory for further analysis using a benchtop Raman spectrometer. Measurement of pH level was conducted using a Semlos digital pH meter, having a resolution of 0.01 and a detectable pH range from 0.00 to 14.00. The calibration medium used was a pH buffer powder solution with pH of 4.01 and 6.86. The HI98501 Checktemp® Digital Thermometer from Hanna® Instruments was used to measure water temperature. It provides high accuracy with a precision of ±0.2 °C and a resolution of 0.1 °C. The device can record temperatures ranging from -50.0 to 150.0°C. The temperature meter was calibrated using the CAL Check™ feature.

2.3. Microbial identification

Microbial identification was conducted using a Raman benchtop spectrometer and the HORIBA LabRAM HR Evolution model. The instrumentation encloses a dual laser input (532 nm and 785 nm) with a power output of 100 mW, a holographic grating with a density of 1800 gr/mm, a backscattered confocal microscope system with a 100 objective, 500 pinholes, and a 200 slit width. A silicon (Si) substrate size of 1 mm×1 mm was used for spectrum calibration, obtaining Raman shift wavenumber and peak intensities at 520 cm^{-1}, whose spectral structures are well-known in literatures. The method of measurements involving Raman mapping technique, scanning nine measurements of different point-to-point on the Raman cross-section water sample to avoid overlook acquisitions. To differentiate contaminated and uncontaminated water samples, Raman spectra for pure water serves as a control variable, were analysed within peaks at wavenumber ranging from 2700 cm^{-1} to 3600 cm^{-1}, corresponding to H_2O molecules. Any distinct peaks present below the specified range, also known as the "fingerprint regions", spanning from 400 cm^{-1} to 1800 cm^{-1}, indicate possible impurities or other substances in the water sample [25]. Microbial species identification using Raman spectrum analysis is based on signature peaks within a range of bands associated with each cell macromolecule monomer, depicting distinctive functional groups [26]. This is due to the vibrational modes (symmetric, asymmetric, and bending) within molecular cell composition, caused by radiation of lights induced by Raman spectroscopy, modifying the molecular structure of species cells. For instance, characterizing spectral signature peaks for monomers of lipids in microbial cells, such as fatty acids, are represented in Raman shift at 1,278 cm^{-1} and 1,746 cm^{-1}, indicating the C=C and C=O stretching molecular patterns [27]. A non-destructive Raman spectroscopy is a powerful method for the detection of microbial contaminants in water environments, offering tremendous advantages over other water quality monitoring method as extensively discussed in [28].

2.4. Data analysis

The OriginPro 8.6 software was used for statistical analysis and interpretation of the distribution patterns for quality measurements collected at residential POUs. The data pre-processing of acquired Raman spectra was also executed. The initial steps for refining the acquired Raman spectrum are wavenumber calibration, band fitting, polynomial smoothing, background correction, and normalization. By comparing unknown acquired spectra to spectra in the database, KnowItAll® initiates a cross-examination search.

3. RESULTS AND DISCUSSION

3.1. Analysis of parameters

Tap water samples were taken in response to seasonal fluctuations, ranging from heavy rain (November 2017 to January 2018) to dry summer (February 2018 to April 2018) weather. Findings showed that almost 2.4% of tap water at residential POU was acidic, below 6.5. Seven water samples were inappropriate for drinking or daily use, and the sample was collected between November 2017 and January 2018. The remaining was within acceptable range of pH from pH 6.24 to 8.58 and temperature from 22.05 °C to 32.15 °C. There were no indications of tap water samples below 6.5 between February 2018 and April 2018, suggesting that all samples within that period are within acceptable value. During the rainy monsoon season (November 2017 to January 2018), the ambient temperature was 28 °C, and the lowest was 22 °C. Meanwhile, the peak and lowest ambient temperatures throughout the dry and sunny seasons (February 2018 to April 2018) were 33 °C and 24 °C, respectively. Ambient temperature was measured on the day of sample collection. From the observation, the average ambient temperature in the rainy season (November 2017 to January 2018) was significantly lower than in the warm and sunny season (February 2018 to April 2018), which could explain the slight pH drop observed at POU locations. Any readings that were not within acceptable ranges for tap water, as provided by environmental agencies, were marked as outliers. Outliers' identification enables the separation of contaminated water samples, which were further used for composition analysis using spectroscopic techniques. These outliers represent actual events, such as spikes in water temperature corresponding to pH drops associated with biological contamination [29]. Acidic water samples in the distribution system tend to have a higher risk of microorganism concentrations caused by faecal contamination, stormwater runoff, waste emissions, and rapid urbanization activities. There is considerable evidence that environmental factors can cause sudden drops in pH levels, resulting in microorganism activity in distribution systems, as supported by other studies [30], [31]. Table 1 presents the extreme pH level and temperature conditions in residential POU locations, including ambient temperature measured during the month of sample collection.

Table 1. Extreme value of pH level below 6.5 at several residential POU locations

Sampling months	Ambient temperature (Hi/Lo), °C	Residential POU locations	Quality parameters	
			pH	Temp. (°C)
November 2017	28/24	L_{H02}	6.27	31.90
		L_{G10}	6.32	29.83
December 2017	26/24	L_{H03}	6.48	29.87
		L_{G09}	6.46	25.60
January 2018	24/22	L_{G11}	6.35	29.88
		L_{G16}	6.24	29.35
		L_{K09}	6.32	28.21

The most acidic water samples were found in POU L_{G16}, having a pH drop of 6.24 at 29.35°C in January 2018 with the lowest ambient temperature. The highest pH was in December 2017, with a value of 6.48 and 6.49 in the POU location at L_{H03} and L_{G09}, respectively. Based on distributional patterns, high water temperature corresponded to low pH values; a similar trend in other findings was also presented previously [32]. These extreme data were isolated for further investigation into its composition to determine whether it contains any biological properties. Low pH and high temperatures in water can indeed trigger bacterial production, but the extent of this effect depends on various factors.

3.2. Raman spectrum interpretation

The identification of characteristic peaks indicates that seven water samples were contaminated with bacteria species known as the gram-negative *Legionella* genus. The preprocessing of Raman spectra using the first derivative and Savitsky-Golay (SG) smoothing technique are shown in Figures 1(a) and (b), respectively. Figure 1(c) displays the Raman spectra for tap water samples that are contaminated at specific POU locations, namely L_{H02}, L_{G10}, L_{H03}, L_{G11}, L_{G16}, and L_{K09}. Each location was depicted using distinct colour codes for the acquired spectra, with shaded regions indicating characteristic peaks for *Legionella* species. The Raman spectra exhibit distinct peaks corresponding to the cellular compositions of macromolecules found in bacterial cells representing polysaccharides, proteins, and nucleic acids [33]. In POU locations L_{G09} and L_{G11}, however, there are slight spectral intensity differences between 1,280 cm^{-1} and 1,320 cm^{-1}. The significant medium-intensity peaks fall around band 1,300 cm^{-1} and gradually weaker peaks at 1,317 cm^{-1}.

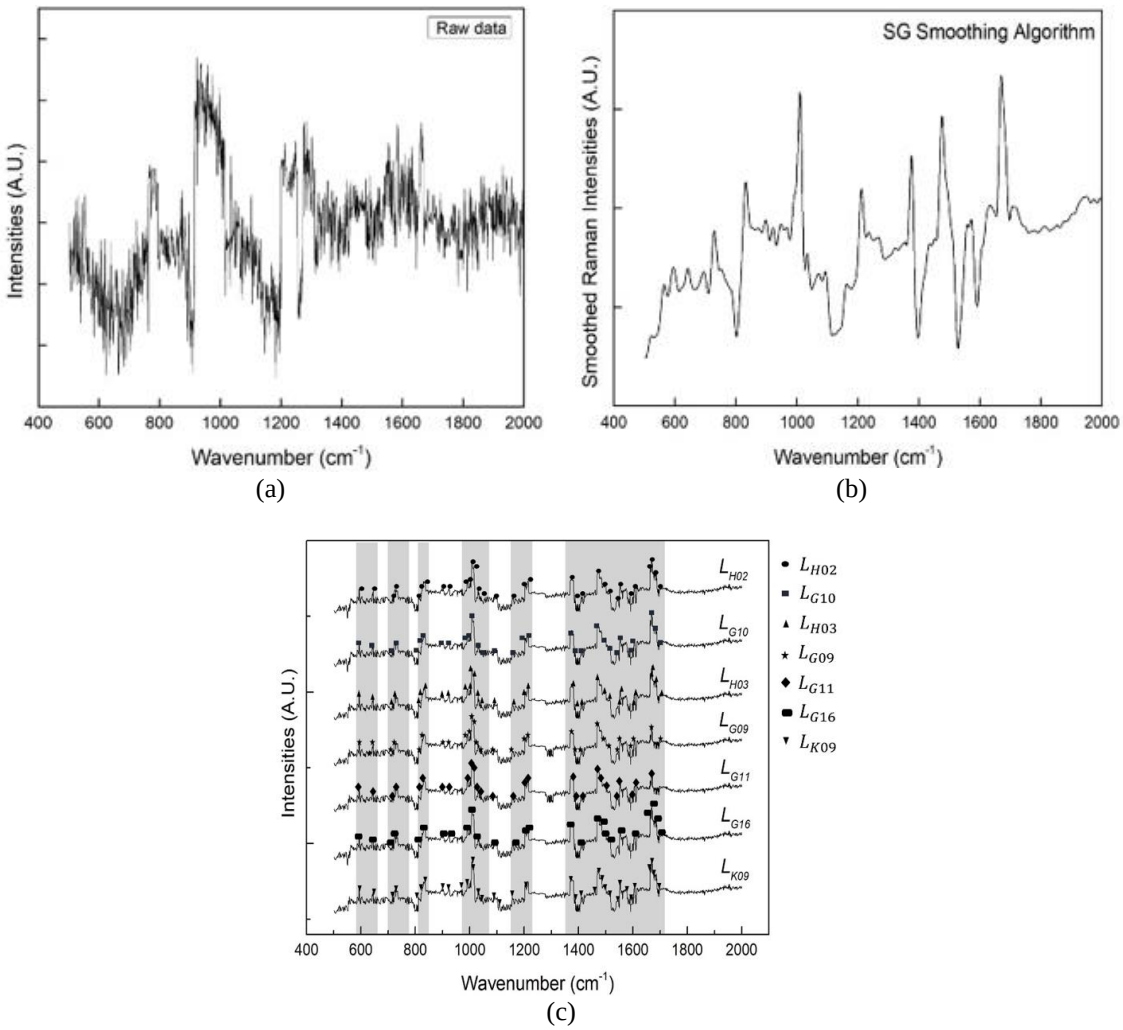


Figure 1. Acquired Raman spectra; (a) raw spectrum, (b) smoothed SG filtering spectrum, and (c) *Legionella* bacteria species in seven POU tap water samples at locations; L_{H02}, L_{G10}, L_{H03}, L_{G11}, L_{G16}, and L_{K09}

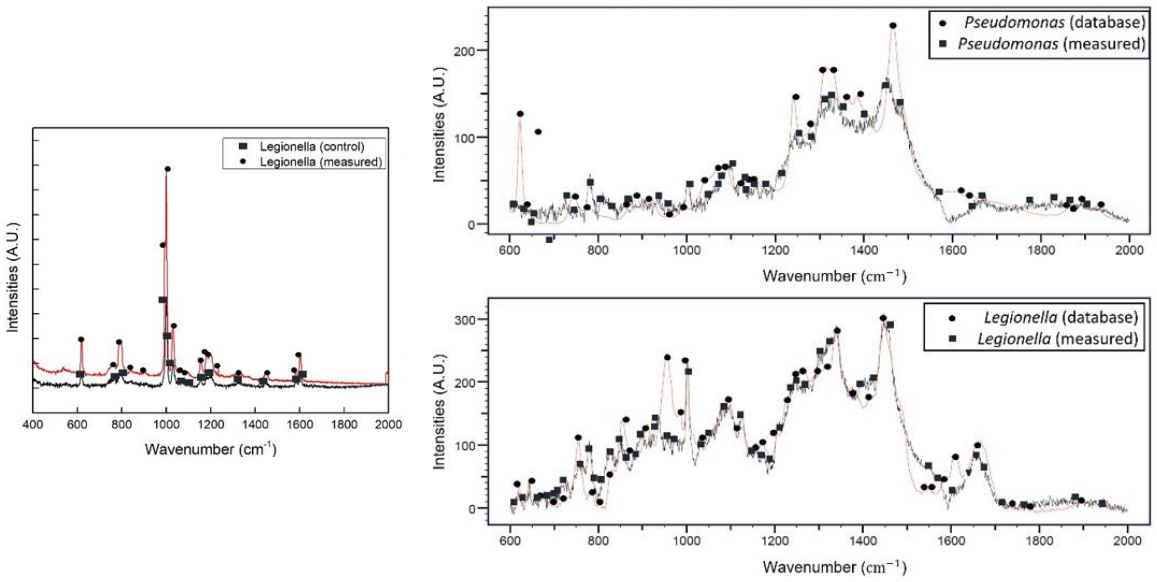
There are subtle variations in the spectral differences within the range of 1,670 cm^{-1} to 1,700 cm^{-1}. The region represents amide molecular vibrations, indicating amide bonds' secondary structures [34]. Precisely, these areas correspond to the amide-type I and III molecular bonds of amino acids. The hydrogen bonding between amino acid residue structures causes differences in absorbance intensities due to differential molecular patterns and geometric orientations [35]. The signature peaks identification was conducted by comparing the acquired Raman shift (wavenumber) to the wavenumber from the Raman band correlation table and previous studies conducted on *Legionella* bacteria identification, as summarised in Table 2. The prominent Raman peaks are seen at wavenumbers of 3,043.8 cm^{-1}, 3,394.34 cm^{-1}, and 3,638 cm^{-1}, suggesting the presence of H_2O bonds, which correspond to water molecules stretching vibrations [36], [37]. The peaks observed at bands 749.37 cm^{-1} and 776.50 cm^{-1} represent polysaccharide compositions in *Legionella* species membrane cells, accommodating to strong C-H stretching vibration signals [38]. Major polysaccharide components in microorganism cell membranes associated with the peak centred around 757 cm^{-1} indicate the presence of xyloglucan chains [39]. The Raman *Legionella* spectrum shows visible peaks at bands 829 cm^{-1} and 892.52 cm^{-1}, representing features of the aromatic amino acid tyrosine. The phenol ring breathing modes and overtone deformation modes are caused by double-bonded aromatic amino acid tyrosine seen in specified bands.

While a Raman correlation table was utilised for identifying specific peaks, statistical correlation analysis was also performed between the two spectra corresponding to each wavenumber to validate Legionella's distinctive peaks further, as shown in Figure 2. Figure 2(a) presents the comparison between Raman spectra measured on contaminated POU tap water samples and the *Legionella* cultivation on an agar plate (control variable). The Pearson correlation analysis was performed to analyse similarities between both

samples by measuring the correlation value, *r*. The absorbance intensities and Raman wavenumber shifts were set as variables used in the correlation algorithm. The Pearson correlation coefficient values between both samples containing *Legionella* bacteria were *r*=0.95127 and *r*=0.95442, which were associated with absorbance intensities and Raman shift, respectively. This indicates a strong correlation between both Raman spectra, indicating high similarities, around 95%, of Raman signature peaks for *Legionella* bacteria in the measured and controlled samples. The KnowItAll spectral database system compares these bacteria to those in the database based on percentage similarities. Figure 2(b) compares database spectra and measured spectra for *Pseudomonas* (data validation) and *Legionella*, having high correlation percentages of 95.13% and 96.81%, respectively.

Table 2. Cross-examination of bands assignment for *Legionella* species Raman spectrum

Measured Raman shift (cm^{-1})	Reference Raman shift (cm^{-1}) [40]-[43]	Molecular vibrations
593.37	593, 560	C-C-O deformation
644.75	640, 690	C-N symmetric
749.37	745, 725	C-H stretching
776.50	778, 776	C-H stretching
829.81	826, 828	Benzene ring
892.52	890, 856	Benzene ring
1,002.65	960, 1004	C-CH_3 formation
1,008.11	1,006, 1,004	Ring breathing
1,030.65	1,031, 1,030	C-OH group
1,226.70	1,236	CH_2 formation
1,378.12	1,380, 1,331	H-C-C, H-C-O, H-O-C
1,482.21	1,480, 1,450	C-H deformation
1,570.91	1,575, 1,578	C=C stretching
1,669.22	1,669, 1,660	C=C stretching



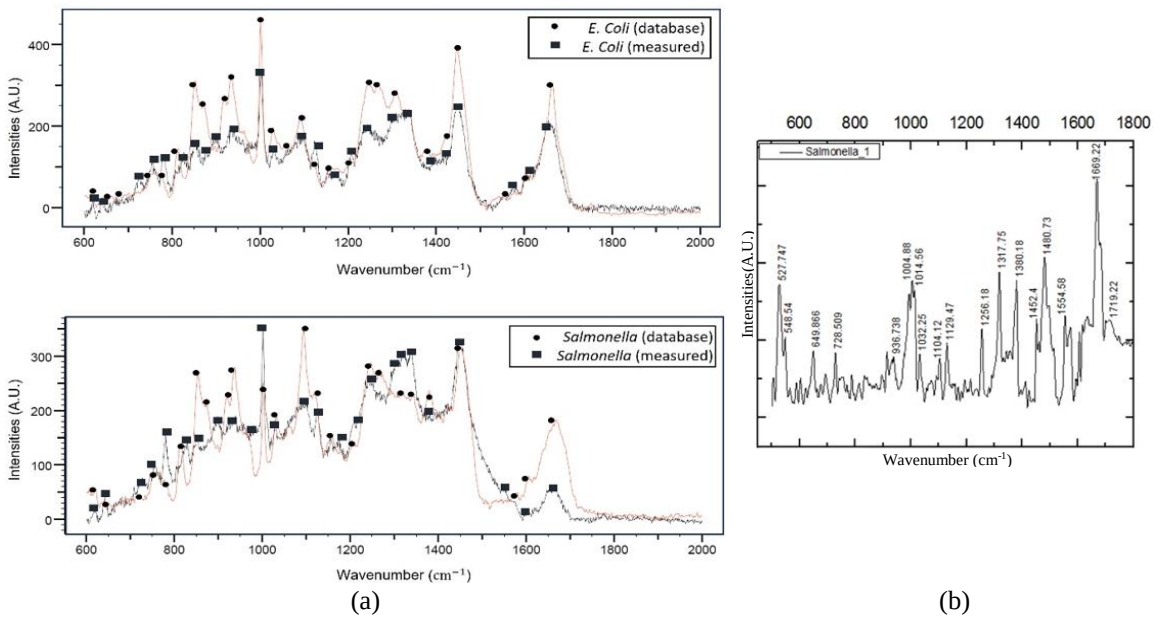
(a) (b)

Figure 2. Comparison of *Legionella*'s signature peaks on contaminated POU tap water samples and the bacteria sample; (a) Raman spectrum for *Legionella* and (b) comparison of Raman spectrum for *Pseudomonas* and *Legionella*

Figure 2(b) illustrate distinct variations in peak patterns between *Legionella pneumophila* and *Pseudomonas* aeruginosa bacteria, which are observable at graph point. The prominent peaks observed at 1,735 cm^{-1} represent the stretching vibration of the C=O double bond in polyhydroxy butyrate (PHB), which is the storage polymer found in *Legionella* cells in tap water. It is worth noting that no such peaks were detected in other bacterial samples. Raman bands are attributed to constituent components of macromolecules commonly found in bacterial cell metabolism. Protein compositions, specifically amide, phenylalanine, and aromatic amino acids, in *Legionella* and *Pseudomonas aeruginosa* species have similar peaks at 1,669 cm^{-1}, 1,238 cm^{-1}, 1,004 cm^{-1}, 856 cm^{-1}, and 828 cm^{-1}.

All pre-stagnation water samples, taken three weeks before semester breaks, had pH levels within the acceptable range. However, the pH levels changed following the post-stagnation water samples, and the water became acidic. Based on this observation, about 15.8% of post-stagnation water samples were not within the acceptable range. Nineteen samples show low tap water quality caused by disrupted water flow and intermittent usage. Water samples collected on the first floor did not contribute to any acidic samples, whilst the majority of those samples were collected on the third floor (42.1%), followed by the fourth floor (36.8%) and the second floor (21.1%). These acidic water samples were further analysed using a Raman spectrometer to identify any possible intrusions. Visually, all tap water shows a clear and transparent appearance. However, observing the physical characteristics of water itself does not dictate its quality condition—the precipitation of samples with a pH of less than 6.5 shows acidity after three weeks of stagnation. Consequently, Raman spectroscopy was able to identify microbial intrusions in a post-stagnation water sample in POU's location, which belongs to the *Salmonella* species, as presented in Figure 3. Similarly, as *Legionella* spectrum, the Raman spectra for *Salmonella* produce diverse peak intensities across wavelength from 600 cm-1 to 1,800 cm-1, signifying the molecular functional groups of microbial cell structures. Based on Figure 3(a), the difference between the ratio of band intensities and Raman shift wavenumber is significant, distinguishing species of *Salmonella* from other bacteria, which, in this study, an *E. coli* spectrum was used.

One of the central peak intensities differences was significant at wavenumber 1,669.22 cm^{-1}, 1,452.4 cm^{-1}, 1,341.54 cm^{-1}, 1,317.75 cm^{-1}, 1,104.12 cm^{-1}, and 1,004.88 cm^{-1} for both spectra. Qualitatively, both spectra also exhibit different graphical visualisations. The correlation method was employed to determine the similarity between two spectra, with a higher dot product value indicating a more remarkable similarity between the measured and Raman database, resulting in a high correlation percentage of 97.49% and 91.63% for both *E. coli* and *Salmonella* bacteria, respectively. The signature fingerprint Raman peak for *Salmonella*, including their band assignments, is shown in Figure 3(b). Within the wavenumber range of 527 cm^{-1} to 1,720 cm^{-1}, numerous discrete bands were observed. Similar to many Gram-negative bacteria species, these bands were assigned as follows: 649.87 cm^{-1} (guanine and tyrosine); 728.51 cm^{-1} (adenine dinucleotide); 936.74 cm^{-1} (C=C and C-N deformation); 1,004.88 cm^{-1} (Phenylalanine); 1,032.25 cm^{-1} (C-C stretching); 1,256.18–1,317.18 cm^{-1} (Amide III); 1,480.73 cm^{-1} (CH_2 deformation); 1,554.58 cm^{-1}(Amide I). For *E. coli* strains, the protein cell structure bands are observed at peak wavelengths of 1,662 cm^{-1}, 1,232 cm^{-1}, 1,005 cm^{-1}, 857 cm^{-1}, and 829 cm^{-1} indicated in Figure 3(a). Similarly, Raman peaks of 1,660 cm^{-1}, 1248 cm^{-1}, 1002 cm^{-1}, and 858 cm^{-1} are found in *Salmonella typhimurium* cells. Another instance of nucleic acids produced through the vibrations of guanine and adenine rings can be observed at peaks approximately 1,578 cm^{-1}, 725 cm^{-1}, and 690 cm^{-1}.



(a) (b)

Figure 3. Raman microscopic image and signature peaks of characteristic bands for *Salmonella* singled-cell bacteria; (a) comparison of Raman spectrum for *E. Coli* and *Salmonella* and (b) Raman spectrum for *Salmonella* (measured)

The distinctive peak at 730 cm^{-1}, which is a characteristic signature for *Salmonella typhimurium* cell serotypes indicates the presence of a diverse array of N-acetyl D glucosamine in the bacterial cell wall, distinguishing it from other organisms' species. The absence of similar peaks in other bacterial samples suggests that there may be unique characteristics or compositions in the storage polymers of *Legionella pneumophila* and the cell wall of *Salmonella typhimurium*. Significant intense spectral peaks can be seen in the wavenumber range of 786 cm^{-1} to 1,575 cm^{-1}, suggesting the composition of nucleic acid in cell membranes, whilst the spectral peaks falls in region 762 cm^{-1} to 1,617 cm^{-1} represents the presence of aromatic amino acids [44]. These biological characteristics are crucial for species identifications, that are indicative of chemical composition in bacterial cells [45]. The persistence of *Salmonella* bacteria in residential and household faucets is a rare event. However, several studies show that these species exist in the distribution system and are linked to food wastage and crop production, eventually reaching POU's area [46]. The findings suggest that Salmonella exists in the residential POU's system because of infrequent usage and water stagnation.

Water samples exhibited elevated acidity levels during the monsoon season, coinciding with low ambient temperature and humidity. This implies that environmental factors have a substantial influence on tap water quality. Moreover, the findings indicate that water quality alteration could potentially be attributed to rainwater run-off and groundwater contamination. The EPA defines biological qualities affected by temperature fluctuations in water bodies as organism survival, growth, reproduction, development, behavior, and habitat preferences [47]. During inclement weather conditions such as storms or rainfall periods, rainwater traverses over exposed terrestrial and aquatic surfaces. Many previous studies have shown significant water ecology impacts derived from rainwater components. These impacts include the discovery of inorganic ion species during monsoon periods [48], chemical compositions [49], and industrial combustions [50]. According to the pH levels found in November 2017, December 2017, and January 2018, seven water samples were not within an acceptable range. Any readings that were not within acceptable ranges for tap water, as provided by environmental agencies, were marked as outliers. These outliers represent actual events, such as spikes in water temperature corresponding to pH drops associated with biological contamination. There is considerable evidence that environmental factors can cause sudden drops in pH levels, resulting in microorganism activity in distribution systems. Depending on the type of bacteria species and acidity tolerance, low pH levels can promote bacterial production and growth. Several bacteria species can withstand acidic water conditions, such as *Streptococcus genus*, *Acidobacterium capsulatum*, *Escherichia coli*, and *Propionibacterium acidipropionici* [51]. Water distribution pipeline networks provide an ideal environment for bacteria to reproduce and a fertile environment for bacterium growth. This is due to several growth-promoting nutrients that allow bacteria communities to survive, even in low-oxygen environments.

3.3. Proposed micro-spectrometer configuration

Each phase of the hardware design process consists of three primary components: the Raman optical setup, the spectrometer system, and the water quality monitoring web server. These components are depicted in Figure 4. Each element consists of crucial criteria used in the development of a comprehensive portable spectrometer integrated with a cloud-based water quality monitoring system. Several design parameters that were considered are Raman optical configurations, materials selection and lens design, diffraction grating and light detector specification. These parameters affect the outcome of Raman spectral resolution and spectrometer sensitivity; therefore, ensuring optimal design parameters is essential. As for the development of a web-based quality monitoring server, it is imperative to ensure overall system performances are satisfactory, particularly in data acquisition time and real-time remote sensing capabilities. The suggested device is small, lightweight, and compact, offering cost-effective on-site measurements that enable remote detection of microorganism contaminants in residential or household pipeline systems, including tap water. With its wireless capability and real-time data transfer using internet of things (IoT) integration technology, this miniature spectrometer simplifies water quality measurements, making them quick and straightforward.

The hardware is designed to align with faucet measurements for tap water. Consideration of pipe widths and waterproofing features is crucial during water sample analysis. The NodeMCU firmware facilitates data acquisition to and from Amazon cloud networks, which are utilized for IoT database management systems. This proposed hardware offers unique features: i) facilitating real-time detection of bacterial contamination events in household water supply pipeline systems, ii) enhancing water quality management for decision-makers, iii) ensuring safety for consumer usage, and iv) enabling both end-users and water stakeholders to synchronize contamination event occurrences. Additionally, it is compact, lightweight, and easy to use. This system includes a detachable customized hollow faucet connection that can be installed on various pipes, such as head showers, toilet faucets, or washing machine water supply. Once water flows through this hollow connector, a mesh separator functions to collect a water sample for testing purposes. To ensure separation from the water sample, the light source and illumination light collection sub-layers are shielded by an uncoated white float window glass (measuring 15 mm×15 mm×3 mm). The

hardware was constructed based on these sub-layers and meticulously aligned to optimize light transmission. The sub-layers were designed using CATIA V5 software, a 3D design platform. Precise measurements were taken for each optical lens, slit aperture, light detector, and other sub-components to ensure perfect alignment within the light transmission path. Subsequently, convex lenses were fixed in position, and reflecting mirrors were placed on an adjustable angle rotator setting. This adjustment ensures that the sensor board receives all light reflected from the surface mirror. Finally, the spectrum sensor board and data transmission module were securely positioned. The performance of the proposed device will be discussed later, and the device's capabilities in monitoring the quality of the water supply at POU's location will be demonstrated.

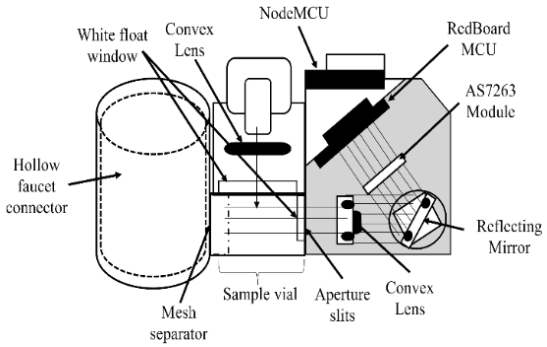


Figure 4. Device architecture for IoT Spectroscopic approach

4. CONCLUSION

In conclusion, detecting bacterial contaminants in household POU environments using the spectroscopy method offers several advantages over conventional approaches in water quality monitoring applications. Raman spectroscopy's ability to identify various microorganism contaminants at POUs significantly improves water quality assessments. The Raman fingerprint recognition enables the detection of a wide range of water pollutants compared to the conventional water quality monitoring approach. Integrating IoT technology with Raman spectroscopy elevates the effectiveness of water quality assessments, expanding its capabilities in detecting targeted pollutants in water ecology. This approach facilitates real-time monitoring, and IoT-spectroscopy offers versatility in various water sources quality monitoring, ensuring a safer water supply. In addition, remote sensing technology enables the detection of real-time events in POU water samples and monitoring changes in water quality over time. As water pollution threatens public health, future studies should focus on improving water quality monitoring techniques to a more compact and efficient approach, ensuring that water policymakers and stakeholders have easy access to real-time quality data. The sensitivity and specificity of these techniques should be improved while addressing challenges to real scenarios of water interferences. Developing a centralized monitoring station of data about distribution system ecosystems similar to data available from POU's location is critical. Consequently, the goal of the process would be to improve the ability to understand, monitor, and maintain what characterizes a healthy microbial community in the distribution system. A shared data platform has another vital benefit; all stakeholders can use the data to design experiments, test hypotheses, evaluate new treatments, and build models, whilst users can provide first-hand information on water quality at the consumption level.

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AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
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R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

CONFLICT OF INTEREST STATEMENT

Authors state no conflict of interest.

INFORMED CONSENT

We have obtained informed consent from all individuals included in this study.

DATA AVAILABILITY

Data availability is not applicable to this paper as no new data were created or analyzed in this study.

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