doi: 10.2166/9781789063714_0223

Chapter 20

Multi-analyte assessment of water quality

*Kamalesh Chaudhari, Vidhya Subramanian and Thalappil Pradeep**

Department of Chemistry, Indian Institute of Technology Madras, Chennai, India
**Corresponding author: Pradeep@iitm.ac.in*

ABSTRACT

A thorough water quality assessment requires sample testing for a set of parameters. In field measurements, it is not necessary to precisely determine water composition. Field measurements can be planned only to roughly understand the necessity of in-depth lab-based analysis. This can be done by developing methods that are reagent free, independent of high-end instrumentation, and facilitative of multiplexed detection. While using multiplexed detection techniques, it is necessary to identify hidden signals using a probabilistic/predictive approach. This can be achieved by analysing the data from the measurements using AI and ML-based prediction techniques. The spectroscopy or electrochemistry-based signals exhibit minor sample-to-sample variations, which can be processed with data analytics tools to predict multiple analytes in water. Due to advancements in the miniaturization of sensors and cloud computing-based data analysis technologies, it has become possible to realize such data analysis-based multi-analyte sensing and detection methods.

Keywords: multi-analyte assessment, sensors, water quality, portable devices, predictive analysis

20.1 WATER QUALITY ASSESSMENT

Spatiotemporal variations in water quality are common. These variations are mainly due to differences in the composition of rocks, soil, and changes in seasons across the country (Bengtsson, 2010). In the hydrological cycle, water interacts with the surrounding environment, air, and soil. These environmental properties can either be beneficial or detrimental to water quality. Different human activities and the production of waste also add to the hazardous substances in water, causing further deterioration in its quality. In rural areas, uncontrolled use of fertilizers, improper management of domestic waste, and poor agricultural practices are the sources of contamination in water. In the urban and industrial areas, discard of effluent from production processes, discard of electronic items/batteries, and chemical spills lead to the contamination of surface water with highly toxic chemicals.

A set of quality parameters to be tested in water sample varies according to the source of water and its surroundings. The most common source is the groundwater pumped from aquifers formed by underground rocks and soil. Ground water levels vary according to region, seasonal changes and the amount of rainfall. These impact and contribute to the various complex changes in water quality. Another source of water is surface water, which is available from lakes, ponds, rivers, springs in the mountains, and so on. Once this water is exposed to the open environment and sources of pollution, it becomes unsafe for drinking. Rainwater is a relatively purer source of water as compared to groundwater or surface water. If rainwater is collected directly or from a clean rooftop, it remains clear and free of contaminants. In conclusion, contaminants in water can be grouped and correlated based on water sources and regions (Singh *et al*., 2020).

The presence of contaminants in excess of their permissible limits as set by the Bureau of Indian Standards (BIS) makes the water unsafe for drinking. Water quality can be determined by a set of physical and chemical observations. Such measurements can be performed with portable devices or a set of chemical reagents, even in field environments. In some cases, there are trace level contaminants in water which are invisible and harmful even at ultra-low concentrations (Zamora-Ledezma *et al*., 2021). A few of these can be tested with chemical reagents, and the remaining may require sophisticated instruments. For such measurements, water samples can be collected with BIS-specified protocols and transported to professional laboratories with high-end technologies and facilities. BIS has grouped contaminants into six major groups, organoleptic and physical parameters, substances undesirable in excessive amounts, toxic substances, radioactive substances, pesticide residues and microbial contaminants. While monitoring drinking water quality, microbial contamination is a major concern. Most of the illnesses and deaths that occur from unsafe drinking water are due to the presence of microbes in water (Saravanan *et al*., 2022).

20.1.1 Requirement of multianalyte assessment

As discussed, certain contaminants can be present in a specific region due to environmental issues or human activities. In water quality analysis, only a few crucial parameters are deemed necessary, while the remaining tests may or may not be required, depending on the historical water quality data of the region. Due to temporal variations in water quality, samples need to be tested frequently for multiple parameters. Periodic testing of water can be time consuming and cost intensive. Many of the parameters cannot be tested in the field with portable devices but samples need to be collected and sent to laboratories. The transport of samples can involve additional expenses and the physicochemical state of the sample can change due to time lapse between collection and testing. Such issues can be avoided if techniques can be developed to analyse multiple water quality parameters with the same method in a single measurement (Hara & Singh, 2021; Mao *et al*., 2015). Also, to avoid the need for laboratory measurements, it is necessary to enable water quality measurements in field environment. For optimum accuracy in field measurements, methods which require minimal efforts are necessary. By using multianalyte assessment, the efforts required during measurements can be reduced, the consumption of chemicals can be minimized, and the obtained data can be employed for data analytics to predict the presence of contaminants that are challenging to test otherwise.

20.1.2 Water quality assessment in the field

Testing of water quality at the consumer end is a challenging task. In rural areas specifically, where there are problems such as a lack of local water quality testing labs and poor connectivity, such testing cannot be done on a regular basis. Collection of water samples from scattered locations across the region becomes a tedious job and requires trained resources. Due to the serious health issues created by contaminated water and the absence of any household potability testing device, tap water is normally considered unsafe for drinking. This leads to the installation of household water purifiers and subsequent wastage in the form of reject water. Hence, ingenious but simple-to-use designs for devices to test water quality are required. Also, to localize the variations in the level of contaminant and their trends, it is necessary that portable devices include location tagging. Several devices have been created to analyse either a single contaminant or a group of contaminants, which can be detected through small signal variations in the sensing probe.

Such portable equipment need not be as precise as lab-level equipment, but it needs to be able to roughly measure and indicate the potability of water in field environments, and generate alerts upon the detection of any abnormalities in the water samples. Despite potential interference from varying water composition and predictive data from statistical measurements, multianalyte measurements can still fulfil the water quality assessment needs at the field level.

20.2 MULTIANALYTE METHODS

As discussed in the previous section, water quality parameters can be grouped according to conditions, such as region, source, and physicochemical properties. These environmental conditions and the presence of contaminants in water exhibit high level of correlation in some cases. For instance, in regions affected by arsenic, the occurrence of iron in groundwater can be correlated. Through these correlations, the necessity for a comprehensive water analysis can be eliminated, and only a few selected parameters need to be examined. In the next step, the data obtained from the measurements can be processed for the prediction of correlated parameters which are otherwise difficult to measure in a field environment. Nonetheless, in certain instances, like with wastewater or surface water flowing across a region, the water's composition can be complex and affected by constantly changing chemistry. In such cases, correlations may not be useful.

The methods used for multianalyte assessment need to be free of high-end instrumentation. Major techniques used for the field-level assessment are chemical reagent-based colorimetric assays or potentiometric sensors. In colourimetry, a set of chemical reagents are used to develop a visible colour which can be correlated with the standard colour charts to infer the concentration of contaminants. Due to the discrete nature of colourimetric charts, digital field test kit readers (FTKs) can be used for an accurate measurement. In potentiometric measurements, water samples are exposed to ion-selective electrodes, which can generate a signal in the form of changes in current or potential difference. In techniques such as anode stripping voltammetry (ASV), samples are deposited on a working electrode and then changes in current due to the stripping of ions at different potentials can be used to infer contaminant presence in water. Many sensors based on various principles have been developed in the past. A few examples of the same are provided in Table 20.1.

20.2.1 Limitations of multianalyte methods

Although multianalyte methods seem promising for the collective measurement of multiple contaminants in water, a few drawbacks arise due to the emphasis on simplifying and lowering the cost of measurements. Due to the aforementioned points, the detection efficiency of portable devices is less as compared to lab equipment. In field environment, deconvolution of interfering components is a complex and computationally intensive task. A huge concentration of interfering ions can increase the baseline. Hence, multianalyte methods can be handled well by data analytics tools developed for the grouping of signals obtained from the measurement of samples. However, when data analytics and grouping techniques are used for the detection of contaminants, the values obtained can have error bars and they are mostly predictive in nature. Such probabilistic values can be accurately analysed only by trained resources, whereas for the common public, these readings need be converted into a weighted estimation of an index for the potability of water. Hence in conclusion, multianalyte assessment can be of quantitative use to trained resources, but for common people, it can only be a qualitative binary indication of the potability of water.

Table 20.1 Some of the sensors developed for detecting contaminants in water.

Analyte	Substrate	Sensing Method	Range	References
Copper	2,2′:5′,2″-terthiphene and MWCNTs on Nylon-6 nanofibres	Amperometry	0.65–39 ppm	Lu *et al.* (2019)
Mercury	Thiamine functionalized silver nanoparticles on filter paper	Colourimetry	>0.5 μM	Budlayan *et al.* (2022)
Silver	Modified carbon paste electrode	Potentiometry	1×10^{-5}–1×10^{-1} M	Adeli *et al.* (2022)
Cobalt	Modified poly(vinyl chloride) membrane	Potentiometry	1×10^{-6}–1×10^{-1} M	Özbek *et al.* (2022)
Cadmium and lead	Bismuth nanoparticle@laser-induced graphene on polyimide film	Electrochemical	>0.5 μg/L and >0.8 μg/L	Zhao *et al.* (2022)
Arsenic and mercury	Gold nanoparticles with dithiothreitol – 10,12-pentacosadiynoic acid (DTT-PCDA) and lysine (Lys)	Colourimetry	710–1248 μg/L and 10.77–53.86 μg/L	Motalebizadeh *et al.* (2018)
Fluoride	Cubic ceria@zirconia nanocages	Colourimetry	0.1–5 ppm	Mukherjee *et al.* (2020)
Lead	Black phosphorus (BP) integrated tilted fibre grating	Polarization	0.1–1.5×10^7 μg/L	Liu *et al.* (2018)
Chromium, copper	ZnO quantum dot	Fluorescence	0.0834 and 2.34 μg/L	Khan *et al.* (2020)
Lead	AuNPs/PPy/$Ti_3C_2T_x$	Electrochemistry	5×10^{-14}–1×10^{-8} M	Zhang and Karimi-maleh (2023)
Arsenic	Hydrous ferric oxide	Plasmon resonance	0.6 μg/L	Yasmin *et al.* (2022)

20.3 DATA ANALYTICS IN MULTIANALYTE ASSESSMENT

20.3.1 Clustering methods

Clustering methods are of great importance in multianalyte assessments. Conventional techniques face challenges in detecting noisy readouts and minor signal variations when trace level contaminants are present. Techniques like principal component analysis (PCA) can be utilized to detect multiple components from a single signal spectrum or to predict the presence of trace level contaminants based on the concentration of other major components in the water sample (Mahapatra *et al.*, 2012).

Cluster analysis utilizes various algorithms to process data according to user-defined criteria and form clusters. The conditions for cluster formation can be the distance between data points, and the statistical distributions or the density of data points in the observation space. Selection of the clustering algorithm depends on user interest and parameters that are used to define the cluster. A few examples of cluster analysis algorithms are: K-means method, fuzzy c-mean, self-organizing map (SOM), interval clustering, and so on (Delgado *et al.*, 2021; Vo-Van *et al.*, 2020). The effectiveness of a clustering algorithm is an optimization problem and it is controlled by factors, such as the number of clusters to be formed, function used to find distance between points, density threshold, and so on. Cluster analysis is an iterative process and depends on the selection of initial parameters followed by manual observations till a satisfactory result is obtained.

The prediction of water quality parameters using the measurements of only a few selected parameters requires data processing techniques, such as PCA. This analysis can be treated as a multidimensional problem and PCA can be conducted to find principal components that are independent and contribute to the variance of the system. PCA helps in improving the interpretability of data and thus prevents information loss. Independent principal components can be found only after the processing of large datasets of the measurements collected over a statistical number of samples. Hence, PCA is an adaptive process which can improve when more measurements are added to the data analytics. Following PCA analysis, highly correlated components enable the reduction of measurement quantities and the prediction of other parameters using independent variables (Parinet *et al.*, 2004).

20.3.2 Machine learning and AI

We are in the era of big data. Terms like data science, data analytics, machine learning (ML), and artificial intelligence (AI) are flooding the market, and data are being considered as wealth of the company. Data collected from surveys and measurements can help build predictive models. Data processing can also give more insights about business or scientific understanding (Rubinger *et al.*, 2022). This significantly impacts decisions regarding future preparations, infrastructure management, planning, or scientific problem solving. Data can reveal new or unknown patterns. To briefly distinguish data science and data analytics, data science is a broader branch that focuses on finding new methods of data analysis and the setting up of standard data processing protocols. On the contrary, data analytics is a more specific area which uses the models and data processing protocols developed by data scientists to find the desired outcome.

ML is a subset of AI which focuses on continuous improvements in generating specific outputs based on data fed into an algorithm. ML algorithms enable self-learning and correction of the model using continuous inputs from data. This helps in improving the prediction and understanding of patterns in data to obtain accurate results. Learning algorithms can be trained in various ways. There is supervised learning that uses specific inputs and outputs for training the ML algorithm. The algorithm finds the general rule which connects inputs with a specific outcome. After training, ML algorithms can take inputs from available data and generate an output based on a general rule. These algorithms are also used to filter the data based on experience or rules defined by a user. ML algorithms can be classified as classification algorithms, producing a limited set of values as outputs, based on the type of input. The outcome of a regression-type algorithm can be numerical values within a specified range. Unsupervised algorithms are employed to discover unknown patterns or groupings within the input data, without relying on any predetermined outputs. The data with no defined categories are grouped/clustered based on shared similarities. Cluster analysis is an example of unsupervised learning in which a predesignated criterion is used to classify measurements into subsets. In addition, reinforcement learning techniques are used in the area of ML where outcomes are partially random and partially under the control of a user. These are optimization processes based on dynamic programming, also termed Markov decision process (Geist *et al.*, 2019). AI are data processing algorithms which mimic the human brain in solving problems. These algorithms/codes are written to rationalize the decision-making process for machines. As compared to data science and data analytics, AI is less process intensive and its major focus is on developing predictive models for decision making and forecasting outcomes based on the data at hand.

20.4 MULTI-ANALYTE ASSESSMENT OF WATER QUALITY

20.4.1 Review of the progress so far

Various detection principles have been used for the multi-analyte assessment of water quality. Detectors are selected based on the type of signal generated and the level of accuracy required. These techniques can be label free and can depend solely upon the intrinsic properties (mass, charge, etc.) of the analytes, or they can be based on the way analyte interacts with a sensing element developed to selectively interact and transduce a signal (Magro *et al.*, 2019). Selective sensing elements can be achieved by modifying substrate surfaces with selective ligands or thin film coatings possessing desired chemical properties. Another way to achieve selectivity is by tuning the properties of the sensing element through various processing techniques, making it more responsive to different analytes under different conditions of electric potential, temperature, and so on. In some cases, the same sensing substrate can be scanned through a range of electric potential to detect different analytes. The existing literature (Biyani *et al.*, 2017; Mukherjee *et al.*, 2020) covers a wide range of developments for assessing multiple analytes in water. We have surveyed and summarized a few selected reports in Table 20.2. To combine multiple assays in a miniaturized platform is a challenging task. In many situations this has been done with the help of microfluidic techniques.

An attempt to develop microfluidic device for the detection of multiple toxins was demonstrated. The technique used antibodies relevant to the toxins with a Lab-On-A-Disc (LOAD) platform for the detection of cyclic peptide toxins in marine water (Maguire *et al.*, 2017). Immunoassays can be developed based on the changes in optical properties of different types of probes such as fluorescence or SPR. Due to tunability permitted by carbon-based nanomaterials, their selectivity towards multiple analytes has been explored extensively in the past few decades. A few examples of the same involve studies conducted by our group for the detection of arsenite and relevant groundwater analytes (manganese and iron) using electrochemically reduced graphene oxide (ERGO)-based paper strips (Jana *et al.*, 2022). Several studies have demonstrated the tunability of GO-based sensors for detecting multiple analytes, albeit not in water (Bauer *et al.*, 2021).Variability noted in the responses of sensing elements can be used to collect the signals from complex mixtures and PCA can be used to further separate the components for the sensing of multiple analytes. Such methodology has been demonstrated by Song *et al.* using an array of sensing elements based on polymer-coated nanowires modified with catalytic nanoparticles (Song & Choi, 2015). Other than these, based on intrinsic molecular properties, approaches have been developed with the combination of on-line solid-phase extraction–liquid chromatography–electrospray–tandem mass spectrometry for the detection of 20 pesticides in natural and treated waters. Such techniques have also been demonstrated for the detection of as many as 103 analytes (semivolatile organic compounds (SVOCs)) using GCMS (gas chromatography-tandem mass spectrometry). Another study performed by Hermes *et al.* has shown that LCMS can be used to quantify >150 micropollutants in aqueous samples (Hermes *et al.*, 2018).

Table 20.2 Survey of multianalyte-sensing devices.

Device	Analyte	Methodology	Detection Range / LOD	References
ANDalyze	Pb, Cu, Zn, CD	Fluorescence	LOD – Pb – 2 μg/L, Cu – 0.6 μg/L, Zn – 1 μg/L, Cd – 0.1 μg/L	ANDalyze
DEP-Chip	Cd, Pb, As, Zn, Cu	Differential pulse voltammetry	LOD – Cd – 2.6 μg/L, Pb – 4 μg/L, As – 5 μg/L, Zn –14.4 μg/L, Cu – 15.5 μg/L	Biyani *et al.* (2017)
uMED	Cd, Zn, Pb	Square Wave ASV	LOD – 4 μg/L	Nemiroski *et al.* (2014)
Vitality Plus Australia	Cd, Co, Pb, Cu, Fe, Mn, Hg, Ni, Zn		1–1000 μg/L	Heavy Metal Test Kit–Vitality Plus Australia
HF–38 Fluorimeter	Pb, U, Cu, Hg	Fluorescence	10–3000 μg/L	HF–38 Fluorimeter For Heavy Metals Testing At ACE12
Metrohm 946 Portable VA analyser (SPE)	As, Sb, Bi, Cd, Co, Pb, Cu, Fe, Mn, Hg, Ni, Zn		1–20 μg/L	Metrohm 946 Portable VA Analyzer

Data analytics and related tools have brought a whole new dimension to the information that can be inferred from multianalyte measurements. In complex composition of water, response from the analyte of interest can be separated using PCA analysis. A few examples of such studies in literature are listed here. One of the major benefits of PCA is reducing the number of parameters and sensing hardware which needs to be used for the measurement of water quality or the same required in water management infrastructure. A study from Ortuno and group has shown that PCA combined with a single ion-selective electrode can be used for multi-ion measurements (Cuartero *et al.*, 2017). Another example has shown that PCA can be useful in simplifying the number of parameters required for water resource management with the example of tropical lake system (Parinet *et al.*, 2004). PCA has also been demonstrated for prediction and evaluation of water quality and reliability of monitoring sources.

Apart from PCA-based projections of dependent water quality parameters, cluster analysis can reveal valuable information, primarily to distinguish different components contributing to changes in water quality. Vo-Van *et al.* (2020) have demonstrated a novel clustering algorithm to understand water quality which represents contribution from four different sources. The application of Grey clustering has been demonstrated in understanding the impact of mining operations on water samples collected from various points in the surrounding region (Delgado *et al.*, 2021). An artificial neural network-based technique has been developed to predict the presence of faecal coliform by Asaf *et al.* (Pras & Mamane, 2023). Cluster analysis can also facilitate addressing discrepancies in the collected data. The data collected in intervals due to various sources of errors or poor measurements can be processed using clustering methods such as interval clustering algorithms (ICA) (Wong & Hu, 2013).

20.4.2 The future of multi-analyte assessment

The development of new technologies is being driven by the need to move towards sustainability, reduce resource consumption, and minimize the impact of techniques on environmental pollution. Advancements in microfabrication techniques and a boom in data analytics with the supporting infrastructure of cloud computing are being used increasingly in the development of sensing elements. Lab-on-chip microsensors with readout interfaces from smartphones are becoming popular. An app-based operation and miniature sensing/readout devices are being developed extensively. Mobile operation with smaller form factor allows direct field application of these techniques. Smartphone-based operation and internet connectivity facilitates the application connectivity with cloud for rigorous computation and a quick predictive analysis based on PCA and advanced data analytics tools. Many new technologies developed in this direction are in a state of lab-to-field transition. Large number of such devices have been launched and commercialized in the last decade (Figure 20.1). Given this background, we envision a future where smartphone-incorporated sensors will enable users to easily perform multianalyte assessments of water quality with just a few clicks on an app, and receive an indication of the potability of the water.

20.5 SUMMARY

We started with an introduction of the different levels of technologies available for the testing of water quality parameters. Different levels of water quality testing are performed for water quality assessment from lab, water source to the end user with field assessment. All these have pros and cons in terms of the readout accuracy, transport of samples, and speed of assessment in the task to indicate whether the water sample being tested is potable or if it needs detailed investigation with high-end equipment. With these we discussed a need for the development of multianalyte-sensing technologies. Followed by this we have discussed various sensing principles which can be used to develop multianalyte sensors and how materials can be tuned to support such measurements. We have listed out the risks involved in predictability of dependent parameters and what impact they may have on the common user. Data analytics has found great applications in the area of multianalyte sensor development and inference from the collected data. PCA and clustering tools have been found useful in simplifying the required

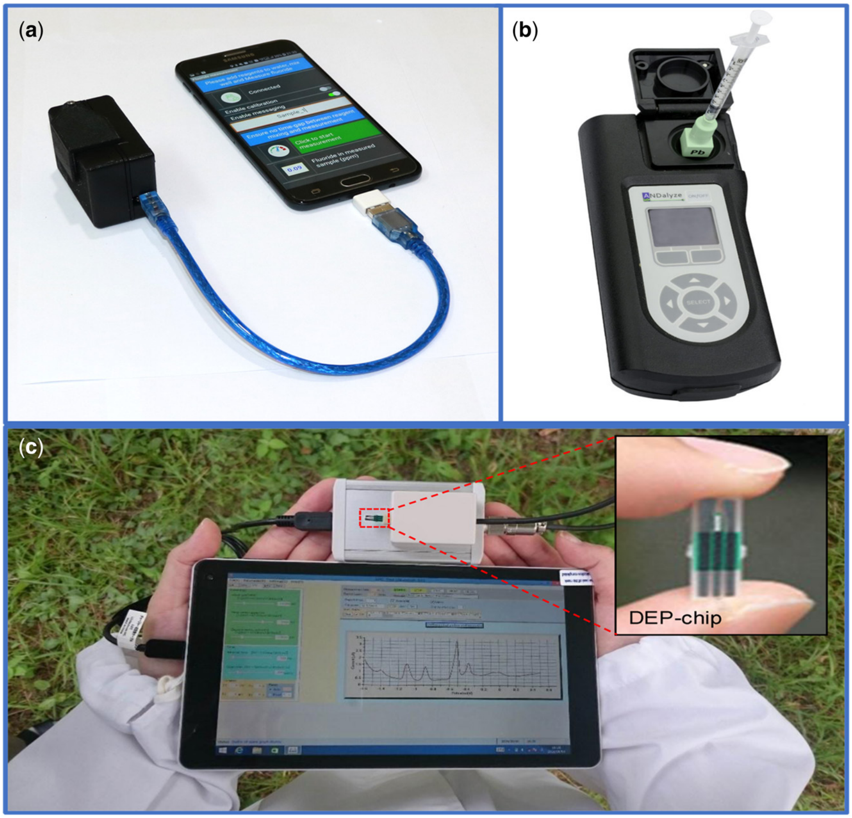

Figure 20.1 Portable devices developed for water quality analysis in field environments. (a) Smartphone based colorimeter for the testing of fluoride in groundwater (Mukherjee *et al.*, 2020). (b) AND 1100 Fluorometer utilised to determine toxicity levels of lead, copper, uranium, mercury, zinc, and cadmium (Reproduced with permission from Alpha Measurement Solutions). (c) DEP-On-Go (Biyani *et al.*, 2017).

multiparametric measurements and understanding different contributions to the water composition. Based on literature survey and an explanation of technical jargon related to area, this chapter can be concluded by looking at the possibility of smartphone-integrated sensors which will be used to indicate potability of water.

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