CORA Cork Open Research Archive
Cartlann Taighde Oscailte Chorcaí

Title	Sensors for chemical contaminants in water
Authors	Barry, Fiona
Publication date	2022
Original Citation	Barry, F. (2022) 'Sensors for chemical contaminants in water', The Boolean: Snapshots of Doctoral Research at University College Cork, 6, pp. 40-45. doi: 10.33178/boolean.2022.1.7
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://journals.ucc.ie/index.php/boolean/article/view/boolean-2022-8 - 10.33178/boolean.2022.1.7
Rights	© 2022, the Author(s). This work is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 licence (CC BY-NC-ND 4.0) - https://creativecommons.org/licenses/by-nc-nd/4.0/
Download date	2026-11-15 13:40:14
Item downloaded from	https://hdl.handle.net/10468/14673

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

THE BOOLEAN
SNAPSHOTS OF DOCTORAL RESEARCH AT UCC

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

Sensors for Chemical Contaminants in Water

Fiona Barry[1,*]

[1] *Tyndall National Institute, University College Cork*
[*] *Corresponding author: fiona.barry@tyndall.ie*

Abstract

Long-term exposure to chemical contaminants in our drinking water can have adverse effects on human health. Such exposure has been linked to cancers, neurological diseases, and cardiovascular diseases. Examples of chemical contaminants found in our water systems include nitrates, heavy metals such as lead, and disinfectant by-products. These contaminants are not visible to the human eye; therefore, it is essential to test the water sample to determine their presence. This work presents an electrochemical sensing platform to detect chemical contaminants in water. This sensing platform has advantages over traditional lab based methods as it eliminates the need to transport samples to a lab by giving at-source, real-time analysis. The sensing component used consisted of two combs of electrodes that were sandwiched together with ultra-small gaps between the opposing combs. This configuration notably enabled the reduction of the sensor footprint by ∼6,000 times compared to previous designs. The significance of this reduction in size means these sensors are lower in cost to produce and require less power to operate. Another benefit of interdigitated electrodes investigated was the ability to use them for *in-situ* pH control. *In situ* pH control was successfully demonstrated using lead. Lead requires acidic conditions for analysis and therefore pH adjusting buffers are typically required for the analysis of lead in tap water which is normally a neutral pH between pH 6 to 8. The ability to electrochemically control the pH of the water sample allowed detection of lead as low as 10 ppb without the need for any additional buffers.

Keywords: Drinking water, chemical contaminants, electrochemical sensor, electrodes, interdigitated electrode array, generator-collector, electrochemical pH control.

Why Do We Care About Chemical Contaminants in Water?

Chemical contaminants in drinking water have been linked to a wide variety of adverse health effects in humans, such as, cancers, neurological diseases, cardiovascular diseases and even miscarriages. Examples of chemical contaminants found in water are inorganic substances

CC BY NC ND

such as nitrates from fertilizer, heavy metals such as lead and disinfectant by-products. Some contaminants enter our water systems by accidental spills, run off from farming activities like spreading fertilizer, while others are introduced during treatment or at the tap. Most chemical contaminants are not visible to the human eye; therefore, it is essential to test the water to determine their presence. Even in cases where they are visible, testing is required to determine which chemical contaminant are present. Current methods of testing use lab based techniques, which require a water sample to be taken, transported to a lab, and then tested on expensive equipment. This process means that only a fraction of the desired water quality analysis can be performed. In my work, I have developed an electrochemical sensing platform that would give at-source testing in a matter of minutes, at lower cost for more widespread analysis.

How Do Electrochemical Sensors Work?

An electrochemical sensor is a device that can give real-time monitoring of chemical contaminants. It operates on the basis that an electrical response (current) is produced at an electrode due to an electrochemical reaction. The electrochemical sensor is placed in the water sample. The chemical contaminant being analysed in the water sample reacts at the surface of the electrode. The reactions that occur are typically redox reactions. This means that the chemical contaminant is either reduced or oxidised. In a reduction reaction an electron (e^-) is gained and in an oxidation reaction an electron (e^-) is lost. This loss or gain of electrons creates an electrical response which allows us to determine how much of the contaminant is present in the water sample. Previous analysis and the chosen electrode/electrolyte system will permit the identification of the contaminant based on the point on the energy (voltage) scale that the reactions occur. This process is illustrated in Figure 1. Here, the chemical contaminant (red) is being oxidised (blue) and the loss of electrons leads to the electrical current. As shown in Figure 1 our electrochemical sensors have several electrodes that are used in the detection of the chemical contaminants; this is known as an array of electrodes. The size of the electrodes in the array is also an important feature, for my work they are on the micron scale. The width of the electrodes is 1 to 2 µm, the length is 25 µm, and the height ranges from 0.35 to 1 µm. To put this in prospective, a human hair which is typically $\sim$50 µm is 25 times wider than the width of these electrodes. The small size of these devices is important as the smaller the electrodes, the less power that is needed to run the sensors. Also, they are cheaper to produce because they use less material. Finally, it makes them easier to integrate into handheld devices or long-term deployable devices for monitoring water systems. In our work we look at ways to further miniaturise the devices while maintaining high performance.

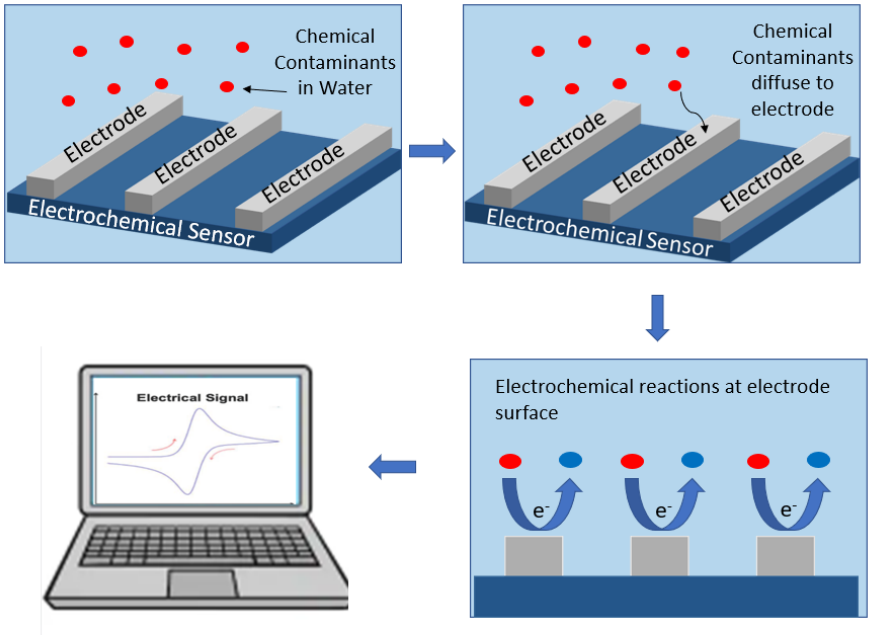


Figure 1: Series of schematics illustrating how reactions occur at electrochemical sensors. The chemical contaminant reacts at the electrode surface where it is oxidised or reduced. This results in a loss (oxidation) or gain (reduction) of electrons. The movement of electrons generates the electrical signal. Source: Fiona Barry.

What's So Special About Our Sensors?

We use electrode arrays in our sensors to help boost the signal so we can detect to very low quantities of contaminants. This is necessary for contaminants such as lead which has a maximum allowable limit in drinking water of 10 parts per billion (ppb). I first set out to define the optimum size and spacing of our electrodes. The distance between the electrodes in the array is important, as we want our devices to be as small as possible while still maintaining good performance. However, in arrays you can't just place the electrodes right beside each other. They need to be spaced at a specific distance away from each other so they can work effectively, deriving benefit from their micron scale and minimising interference. I performed simulations to determine the ideal spacing between our 2 µm wide electrode bands. A layout and brief description of what is happening during these simulations is highlighted in Figure 2(a), where d is the distance between the electrodes, which is varied in the simulations. In Figure 2(b) the electrodes are spaced 10 µm apart. The red represents the uniform concentration of the contaminant in the bulk solution and the blue is the oxidised version of the chemical contaminant that has reacted at the surface of the electrodes and is now diffusing away from the electrode. When the blue area around each electrode overlaps as shown in Figure 2(b) we are not utilising the benefits, instead of acting as individual micro-electrodes, the array is acting as one large electrode which cannot detect to the same limits. This occurs because the electrodes are all competing for the same chemical contaminants and as a result the output current is lowered. The simulation shown in Figure 2(c) shows a more optimal set-up, where the electrodes are

spaced 100 µm apart. Here, there is no competition between the electrodes, and we get the boosted signal we expect from using a microelectrode array.

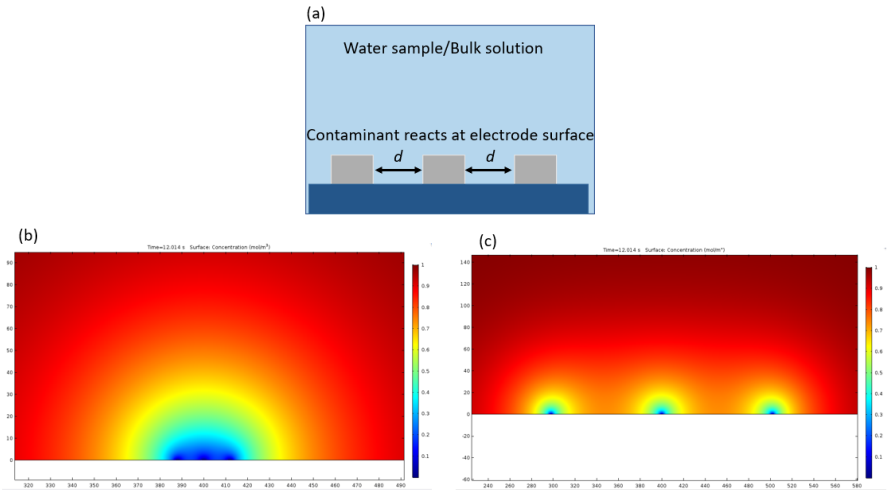


Figure 2: Simulations of reactions at electrode arrays. (a) Brief description of simulation conditions and electrode layout, (b)simulation where electrodes have a 10 µm gap, and (c) simulation where electrodes have a 100 µm gap. Source: Fiona Barry.

Requiring this amount of space between electrodes in an array can greatly increase the overall size of the device. To overcome this, we use an interdigitated electrode configuration. This is where a second comb of electrodes is introduced between the existing electrodes and can be controlled separately, as shown on the overview image (a) in Figure 3. The interdigitated electrode configuration is generally known as a Generator Collector arrangement (GC), as highlighted in Figure 3. In GC electrodes, the redox reaction of the chemical contaminant occurs at the generator electrode while the parameters at the collector allow it to collect all the reduced or oxidised species created and convert them back to the original chemical contaminant form. This is known as a redox loop and can help boost the signal of the sensors by increasing the amount of chemical contaminant available for reaction at the generator electrode.

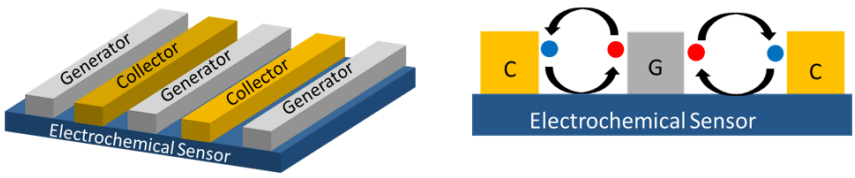


Figure 3: Schematic diagrams of interdigitated (GC electrodes) in top view (left) and cross-section view (right). Source: Fiona Barry.

Simulations demonstrating how GC electrodes operate are highlighted in Figure 4. In these simulations the electrodes are 2 µm in width and spaced 2 µm apart. In the simulation on

the left where the collector electrode is not in use, we can see that the blue area or the oxidised chemical contaminant is overlapping, as shown earlier when electrodes are not spaced far enough apart. The simulation on the right is where the collector electrode has been switched on and is collecting all the reacted chemical contaminant and oxidising or reducing it back to its original form for reaction at the generator. Here, the redox loop created by the collector electrodes not only boosts the signal but also acts like a barrier preventing the blue reacting chemical contaminant overlapping with the neighbouring electrode. This means we can place the electrodes in the array much closer together without overlapping and the redox loop boosts the signal further!

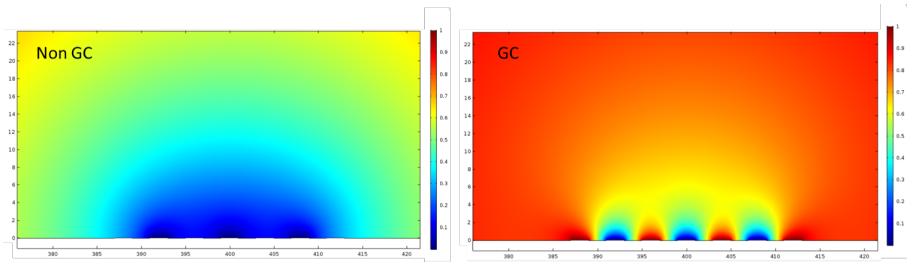


Figure 4: Simulations of GC electrodes where the collector is not in use (Non GC, left) and in use (GC, right). Source: Fiona Barry.

Using these interdigitated GC electrodes, we were able to reduce the size of our electrode arrays by ∼6,000 times while the signal improved by 5 times. By reducing the size of the sensor, we have greatly reduced the power required to use it. So, we have made a more sensitive sensor that is not only smaller but also requires less power to operate.

Bonus Feature!

Interdigitated arrays can also be used to electrochemically change the pH of a solution. The ability to control pH is important for some chemical contaminants, such as lead, as an acidic pH is favourable for analysis. To lower the pH of water to acidic conditions, we use the collector electrode side of the array to split water. In that reaction H_2O is broken down into the individual components, oxygen (O_2) and hydrogen (H_2).

$$2H_2O \longrightarrow O_2 + 4H^+ + 4e^-$$

The H^+ released when the water is split reduces the pH close to the electrodes. Drinking water from our taps in Ireland is generally at a neutral pH of between 6 to 8. The release of H^+ from splitting the water can readily bring the pH down to 3. This is a simplified means to change the pH without additional reagents and as lead undergoes the redox reaction preferentially at lower pH this boosts sensitivity. Using this technique, I have been successful in detecting lead down to 10 ppb in tap water which is otherwise not possible without the use of additives. This greatly simplifies the method for detecting lead and allows for easier at-source detection.

To Conclude

In this work I have designed electrodes that have greatly reduced the size, power consumption and sensitivity of the sensors. These sensors have been used successfully to detect lead in water without the need for additives or buffers. This is advantageous over current laboratory methods as it allows at-source detection and reduces the time and expense that would usually be incurred for testing tap water for lead and other chemical contaminants.

Acknowledgements

Thanks to my supervisor Dr James Rohan and co-supervisor Dr Lorraine Nagle for their continued support. Thank you to Dr Ian Seymour and Benjamin O'Sullivan for their patience and help with my simulations and pH control. Thank you to all my colleagues in Tyndall who helped with this research in some way or another.

Declaration of Interests

This research was funded by Science Foundation Ireland.